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Battelle Columbus Labs., OH

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GC/MS ANALYSIS OF ORGANICS IN DRINKING WATER CONCENTRATES AND ADVANCED WASTE TREATMENT CONCENTRATES

Volume 1

Analysis Results for 17 Drinking Water, 16 Advanced Waste Treatment and 3 Process Blank Concentrates

by

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Contract No. 68-03-2548

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16. ABSTRACT

The goal of this research program was to provide a detailed chemical characterization of organic material concentrated from large volumes (1,500 liters to 15,000 liters) of finished drinking water (DW) and finished water from advanced waste treatment (AWT) plants. The approach used was organic compound identification based on glass capillary gas chromatography-mass spectrometry (GC-MS) analysis of the fractionated concentrate. The purpose of the research program was to enable EPA scientists to correlate the results of the detailed chemical characterization with those from other research programs testing the potential biological activity (i.e., mutagenicity) of the concentrates. Fifteen DW concentrates, sixteen AWT concentrates and five concentrate production method blanks were analyzed.

The cities represented by the DW samplings were Cincinnati, Miami, New Orleans, Ottumwa (Iowa), Philadelphia and Seattle. Most of the unrecovered organic portion and the extracted material not amenable to GC-MS analysis appeared to be humic substances. In the 15 DW concentrates, 1091 organic compounds were identified in a total of 2383 detection instances.

The AWT plans sampled were located at Escondido, Lake Tahoe, Orange County and Pomona (all in California), Dallas, and Washington, D.C. (Blue Plains site). In the 16 AWT concentrates, 991 organic compounds were identified in a total of 2097 detection instances.

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FOREWORD

The many benefits of our modern, developing, industrial society are accompanied by certain hazards. Careful assessment of the relative risk of existing and new man-made environmental hazards is necessary for the establishment of sound regulatory policy. These regulations serve to enhance the quality of our environment in order to promote the public health and welfare and the productive capacity of our Nation's population.

The complexities of environmental problems originate in the deep interdependent relationships between the various physical and biological segments of man's natural and social world. Solutions to these environmental problems require an integrated program of research and development using input from a number of disciplines. The Health Effects Research Laboratory, Research Triangle Park, NC and Cincinnati, OH conducts a coordinated environmental health research program in toxicology, epidemiology and clinical studies using human volunteer subjects. Wide ranges of pollutants known or suspected to cause health problems are studied. The research focuses on air pollutants, water pollutants, toxic substances, hazardous wastes, pesticides and non-ionizing radiation. The laboratory participates in the development and revision of air and water quality criteria and health assessment documents on pollutants for which regulatory actions are being considered. Direct support to the regulatory function of the Agency is provided in the form of expert testimony and preparation of affidavits as well as expert advice to the Administrator to assure the adequacy of environmental regulatory decisions involving the protection of the health and welfare of all U.S. inhabitants.

The purpose of this research program was to enable EPA scientists to correlate the results of the detailed chemical characterization with those from other research programs testing the potential biological activity (i.e., mutagenicity) of the concentrates.

F. Gordon Hueter, Ph.D.
Director
Health Effects Research Laboratory

ABSTRACT

The goal of this research program was to provide a detailed chemical characterization of organic material concentrated from large volumes (1,500 liters to 15,000 liters) of finished drinking water (DW) and finished water from advanced waste treatment (AWT) plants. The approach used was organic compound identification based on glass capillary gas chromatography-mass spectrometry (GC-MS) analysis of the fractionated concentrate. The complex organic concentrates were partitioned into less complex fractions by liquid-liquid partitioning, methylation of acidic components and fractionation of neutral species on silica gel. The purpose of the research program was to enable EPA scientists to correlate the results of the detailed chemical characterization with those from other research programs testing the potential biological activity (i.e., mutagenicity) of the concentrates. Fifteen DW concentrates, sixteen AWT concentrates and five concentrate production method blanks were analyzed.

The cities represented by the DW samplings were Cincinnati, Miami, New Orleans, Ottumwa (Iowa), Philadelphia and Seattle. For DW concentrates, only 20 percent of the organic material in the concentrates for a given sampling was recovered in analyzed fractions, and only one half of that material was of a chemical type suitable for GC-MS analysis. Most of the unrecovered organic portion and the extracted material not amenable to GC-MS analysis appeared to be humic substances. In the 15 DW concentrates, 1091 organic compounds were identified in a total of 2383 detection instances.

The AWT plants sampled were located at Escondido, Lake Tahoe, Orange County and Pomona (all in California), Dallas, and Washington, D.C. (Blue Plains site). Less humic material was present in the AWT concentrates with the result that about 50 percent of the organic material was recovered in the GC-MS analyzed fractions. In the 16 AWT concentrates, 991 organic compounds were identified in a total of 2097 detection instances.

The GC-MS data were surveyed by computer for 53 compounds which might have health effect significance. For DW concentrates, 31 of these compounds were found to be present in a total of 108 detection instances. For the AWT concentrates, 33 compounds were found in a total of 117 detection instances. The DW concentrates uniformly exceeded the AWT concentrates in containing more and higher concentrations of materials attributable to either pollution from the organic chemical industry or consumer use of products containing chemicals. This difference was probably due to the use of granular activated carbon (GAC) or reverse osmosis RO as a final treatment step in the AWT plants but not the DW treatment plants. All DW samples contained some indicators of water re-use (i.e., drugs or metabolites) ranging from very slight (Seattle) to substantial (Miami).

Small volume samples (10 to 30 liters) were also analyzed to study the effectiveness of the RO and GAC treatments in retaining organic molecules. These results together with some of the DW concentrate results indicate that RO membranes do not effectively retain apolar organic molecules.

This report was submitted in fulfillment of U.S. EPA Contract 68-03-2548 by Battelle Columbus Laboratories and covers the period June, 1977 to November, 1980. Work was completed as of November, 1980.

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ABBREVIATIONS AND SYMBOLS

ABBREVIATIONS IN THE TEXT
(See also, Appendix B)

AWT — advanced waste treatment
BOD — biological oxygen demand
CA -- cellulose acetate (RO membrane)
CAS — Chemical Abstracts Service
COD — chemical oxygen demand
DFTPP — decafluorotriphenylphosphine
DW — drinking water
EICP — extracted ion current profile
FC-43 — perfluorotributylamine
GAC -- granular activated carbon
GC — gas chromatography
GC-FID — GC analysis with flame ionization detection
GC-MS -- gas chromatography-mass spectrometry
GSRI — Gulf South Research Institute
HEB -- hexaethylbenzene
HERL-CI -- Health Effects Research Laboratory, U.S. EPA, Cincinnati, Ohio
IFSS — data acquisition program for the System/150 GC-MS data system
IS — internal standard
K-D — Kuderna-Danish, solvent evaporation apparatus
m/e — mass (atomic mass units) to charge (electronic charge units) ratio
μg/l -- microgram per liter
ng/l — nanogram per liter
NTIS — National Technical Information Service
NYL — nylon hollow fiber (RO cartridge)
ppb -- part per billion (1 μg/l)
ppt — part per trillion (1 ng/l)
RF — response factor
RO -- reverse osmosis
RS — relative size; a designator of the size of GC-MS peaks relative to the internal standard, HEB
SGCSM — standard GC separation mixture
SIS — selected ion search; an EICP computer program
SP1000 — a polar GC liquid phase consisting of Carbowax 20M (polyethylene glycol) terminated with nitroterephthalic acid
SP2100 — a nonpolar GC liquid phase consisting of methylsilicone fluid
TOC — total organic carbon

ABBREVIATIONS AND SYMBOLS (Continued)

XAD-2 -- a macroreticular adsorption polymer of polystyrene/2% divinylbenzene copolymer, Rohm and Haas Co.

THREE-DIGIT CONCENTRATE CODE IN THE TEXT AND COMPUTER-PRINTED TABLES

DW Concentrates

M2C — Miami, Florida, combined solvent extract, 2/3/76
M2X -- Miami, Florida, XAD-2 extract, 2/3/76
N2C -- New Orleans, Louisiana, combined solvent extract, 1/14/76
N2X — New Orleans, Louisiana, XAD-2 extract, 1/14/76
O2C -- Ottumwa, Iowa, combined solvent extract, 9/10/76
O2X — Ottumwa, Iowa, XAD-2 extract, 9/10/76
P2C — Philadelphia, Pennsylvania, combined solvent extract, 2/10/76
P2X -- Philadelphia, Pennsylvania, XAD-2 extract, 2/10/76
S2C — Seattle, Washington, combined solvent extract, 11/5/76
S2X — Seattle, Washington, XAD-2 extract, 11/5/76
T1C -- Cincinnati, Ohio, combined solvent extract, 10/17/78
T1X -- Cincinnati, Ohio, XAD-2 extract, 10/17/78
T1Y -- Cincinnati, Ohio, direct XAD-2 extraction, 10/17/78
T4C -- Cincinnati, Ohio, combined solvent extract, 1/14/80
T4X -- Cincinnati, Ohio, XAD-2 extract, 1/14/80
V1C -- Poplarville, Mississippi, combined solvent extract, 3/2/79
V1X -- Poplarville, Mississippi, XAD-2 extract, 3/2/79

AWT Concentrates

B1M — Blue Plains, Washington, D.C., 9/19/74, CH_2Cl_2 extract, cellulose acetate RO brine
B1N — Blue Plains, Washington, D.C., 9/19/74, CH_2Cl_2 extract, acidic cellulose acetate RO brine
B2C -- Blue Plains, Washington, D.C., 5/29/75, combined solvent extract
C1P -- Pomona, California, 9/25/74, pentane extract, cellulose acetate RO brine
C1M -- Pomona, California, 9/25/74, CH_2Cl_2 extract, acetate RO brine
C1N -- Pomona, California, 9/25/74, CH_2Cl_2 extract, acidic cellulose acetate RO brine
C2N -- Pomona, California, 10/2/74, CH_2Cl_2 extract, acidic cellulose acetate RO brine
C3C -- Pomona, California, 6/17/75, combined solvent extract
D2N — Dallas, Texas, 12/10/74, CH_2Cl_2 extract, acidic cellulose acetate RO brine
E1C — Escondido, California, 7/8/75, combined solvent extract
L2P — Lake Tahoe, California, 10/24/74, pentane extract, cellulose acetate RO brine
L2M -- Lake Tahoe, California, 10/24/74, CH_2Cl_2 extract, cellulose acetate RO brine
L2N — Lake Tahoe, California, 10/24/74, CH_2Cl_2 extract, acidic cellulose acetate RO brine

THREE-DIGIT CONCENTRATE CODE IN THE TEXT AND COMPUTER-PRINTED TABLES (Continued)

AWT Concentrates (Continued)

L2D -- Lake Tahoe, California, 10/24/74, CH_2Cl_2 extract, acidic cellulose acetate RO brine
R1C — Orange County, California, 1/27/76, combined solvent extract
R2C — Orange County, California, 2/3/76, combined solvent extract

Blank Concentrates

T2B -- XAD-2 resin elution with diethyl ether
X1C -- evaporated extraction solvent (pentane and methylene chloride)
X1X -- XAD-2 resin elution with ethanol

ABBREVIATIONS IN THE COMPUTER-PRINTED TABLES

CAS NO. -- numbers with five or more digits: Chemical Abstracts Service compound registry number; numbers with four or fewer digits are Battelle numbers

MW — molecular weight
DW — drinking water
AWT — advanced waste treatment
T4 -- data set for samples reported in Volume 3
T5 -- data set for samples reported in Volume 3
RS -- relative size; a designator of the size of GC-MS peaks relative to the internal standard, HEB

SYMBOLS IN THE COMPUTER-PRINTED TABLES

The following four symbols may appear to the left of the compound name:

* — designates a compound on the list of 53 compounds (see Table 4, Volume 1) for which the GC-MS data was specifically searched
+ -- designates a compound which is on EPA's Consent Decree Priority Pollutant list (semi-volitile compounds)
$ — designates a compound which is on the Chemical Indicators of Industrial Pollution list (Federal Interium Primary Drinking Water Regulations, February 9, 1978)
% — designates a compound which is an entry in the EMIC database of compounds on which bioactivity data is available from Oak Ridge National Laboratory

BRIEF DESCRIPTION OF ALL VOLUMES OF THE FINAL REPORT

There are three volumes of this Final Report on EPA contract 68-03-2548. Each is briefly described below and the Tables of Contents of Volumes 1 and 3 are reproduced in Appendix B.

VOLUME 1

Volume 1 covers all aspects of analysis of the concentrates produced from large volumes (greater than 1415 liters (400 gallons)) of drinking water (DW) and advanced waste treatment (AWT) water. Eight key computer-printed tables which show organic compound identification results in integrated listings for the related sets of concentrates (DW and AWT) are contained in Volume 1. All discussion of the analysis results for large-volume DW and AWT concentrates as well as a complete description of the analytical scheme, computerized data management and accounting of all contract deliverables are contained in Volume 1.

VOLUME 2

Volume 2 contains 22 computer-printed tables which comprise the complete set of compound identification results covering the DW and AWT large-volume concentrates. Eight of these 22 tables are also incorporated in Volume 1 as the "core" set of information. The 14 computer-printed tables of Volume 2 which do not appear in Volume 1 provide the following additional information:

1. Identification status (confirmed or tentative) for all instances of compound identification in concentrates.
2. Systematic names, molecular formulas and molecular weights of all identified compounds.
3. Functional group information for each concentrate showing the total relative size values for each functional group on each of the two GC columns (SP1000 and SP2100).

VOLUME 3

Volume 3 covers the analysis of all small volume (10 to 30 liters) samples. These samples comprise the following sets:

1. A group of 13 samples of DW associated with granular activated carbon (GAC) contact treatment using unit "A" at the Cincinnati Waterworks.

2. A group of 7 samples, analogous to No. 1, above, associated with GAC contactor unit "D".
3. A group of 9 samples produced to monitor the reverse osmosis processing of DW sampled at Jefferson Parrish (New Orleans) Louisiana.
4. A group of 4 10-liter samples consisting of two reagent water blanks and two Cincinnati DW samples of which one was processed by lyophylization.

All of the compound identifications results for the above four sets of samples are presented and discussed in Volume 3. In addition, the modified analytical scheme used for these samples is presented in detail and compared to that used for the large-volume samples (Volume 1).

ACKNOWLEDGMENTS

Through the course of this three-year research program, many members of Battelle's technical staff have made significant contributions to the high quality of the results that were obtained. Denis C.K. Lin deserves special recognition for his major contribution to the conceptualization and development of the analytical scheme, results report format and computerized management of the extremely large database. His incorporation of glass capillary GC columns and a large number of deuterated internal standards were definitely "state of the art" at that time (1977). Other Battelle scientists and their contributions to this work include:

Laurence E. Slivon--Design and validation of the computer search and quantification capability; System/150 to INCOS data transfer; EPA/NIH/NSRDS library search implementation; high-density 9-track taping of GC-MS data; numberous utility programs for System/150; mass spectral data interpretation

Bruce A. Petersen--Analytical scheme design, quality control development, and mass spectral data interpretation

Roderick G. Warren--Implementation of the NUCLEUS data management and report production systems

Roger L. Foltz and Richard M. Thompson--Mass spectral data interpretation

Susan G. Watson--Confirmation of compound identification and mass spectral data interpretation

Timothy L. Hayes--GC-MS data processing, 10-liter extraction, data acquisition

Vanessa R. Goff--GC-MS data acquisition, quality control, and mass spectral data interpretation

Denise A. Contos--Concentrate partitioning, residue weight determinations, standards preparation, sample analysis tracking, and GC-MS data searching and quantification

Daniel G. Aichele--NUCLEUS system interaction and operation, report generation and coordination

Patricia P. Kelley--Report system development and production, NUCLEUS interaction

Joseph P. Tabor--GC-MS data screening for artifacts

Cynthia A. Schweiger and Bruce E. Urbschat--Assistance with NUCLEUS operations

The author, as senior team member in the early stages and principal investigator since 1979, was involved in all of the above cited activities except the development of System/150 operation programs.

SECTION 1

INTRODUCTION

Assessing the health effects of trace (part per billion, ppb) levels of organic material in water is an important, if not determining, factor in establishing maximum permissible contamination levels for drinking water (DW) and finished water from advanced waste treatment (AWT) plants. The issue of trace level organic chemical contamination of DW will continue to receive major emphasis in pollution health effect research. However, in the western states, potable usage or other high quality usage of AWT finished water is certain to assume a major role. Pilot and production scale AWT plants are already providing high quality water for use in ground water injection--either to prevent sea water intrusion into coastal aquifers or simply as aquifer replenishment. In addition, direct potable reuse of AWT finished water is now in the planning stages for some municipalities for which unlimited supplies of fresh surfacewater or groundwater are not presently assured. With respect to potential health effects, detection and control of trace level organic contamination in these AWT reuse waters is obviously important for the ultimate protection of DW sources.

The Health Effects Research Laboratory of the U.S. EPA in Cincinnati, Ohio (HERL-CI) is pursuing a research program to characterize the trace level organic materials in DW and AWT water, and to test the biological activity of these materials as an indication of their potential health effects. Ongoing work in the HERL-CI laboratories as well as other research projects contracted through HERL-CI has been concerned with the biological testing of the organic concentrates. The goal of Battelle's research effort under EPA Contract 68-03-2548 has been to characterize the organic materials present in sufficient detail to enable EPA to correlate the compound identification results with the biological test results. This correlation may suggest which of the organic compounds, or classes of compounds, have sufficient potential health effect significance to warrant future regulation and/or monitoring.

In HERL-CI's approach to this research problem, large quantities (1500 to 15,000 liters) of DW and AWT water were concentrated, principally by reverse osmosis techniques, to yield gram-quantity amounts of concentrated organic material. The concentrate production work was performed by another contractor (see Section 4). Eighty percent of each organic concentrate was reserved for biological testing. Half of the remaining 20 percent was analyzed for organic compounds by glass capillary gas chromatography-mass spectrometry (GC-MS). Thus, the sample aliquot analyzed represents between 150 and 1500 liters of the original water for a theoretical concentration factor of 150,000:1 to 1,500,000:1. This extremely high concentration factor, coupled with fractionation of the sample into five separately analyzed organic polarity groups (thereby adding another order of magnitude to the concentration factor), allowed for a more detailed characterization of the portion of organic material amenable to GC-MS analysis in these clean waters than any previous approach. Theoretical sensitivities for some identified compounds reached below the 0.1 part per trillion, ppt, level (0.1 nanogram per liter).

The following is a brief description of the analytical scheme employed:

- Fractionation of the concentrate into five different polarity groups
- Glass capillary GC-MS analysis of four of the fractions on two different GC phases with all generated data archived on 9-track magnetic tape
- Residue weight analysis of the unpartitioned concentrate and the five fractions
- Attempted identification based on mass spectra of all chromatographic peaks and shoulders in the GC-MS data
- Automated searching of GC-MS data files for 53 high-interest compounds and quantification of those found
- Confirmation of tentative identifications by comparison with GC-MS data generated from commercially obtained reference compounds
- Entry of compound identification results and other pertinent concentrate information into Battelle's mainframe computer for automated data management and generation of tabular listings of results
- Concentrate analysis report generation.

SECTION 2

CONCLUSIONS

The results of this research program have shown fractionation of complex organic concentrates followed by glass capillary GC-MS analysis enables the identification of hundreds of organic compounds present in these samples. Moreover, the use of concentration techniques in which thousands of liters of water are used to produce the analyzed sample together with computerized GC-MS data searching have enabled theoretical sensitivities toward individual pollutant species which extend well below the part per trillion (nanogram per liter) level. Thus, results of this research have produced chemical characterizations of very clean drinking waters and advanced waste treatment finished waters in greater detail than previously possible.

The results for drinking water (DW) provide the following conclusions:

- Most of the organic material in the analyzed concentrates consisted of humic-related substances which are not amenable to GC-MS analysis. On the average, more than 90 percent of the organic material present in the concentrates was not recovered through the fractionation scheme. Part of the recovered material is not suitable for characterization by GC-MS analysis, and it is estimated that only 30 to 60 percent of the material recovered into fractions (i.e., 3 to 6 percent of the original concentrates) can be characterized by GC-MS analysis.
- All of the DW sampled (except one case which served as a blank) contained many identified organic compounds, generally between 150 and 400 different species.
- The species identified at the highest levels and greatest numbers were non-aromatic and aromatic carboxylic acids.
- All DW concentrates contained some evidence of the presence of re-use water via the identification of drug metabolites and other materials expected to originate from domestic sewage. The level of re-use water ranged from very slight for Seattle to a significantly high level for Miami.
- All DW concentrates showed some evidence for contamination by organic compounds from industrial discharges (organic solvents and chemical industry commodities, intermediates and wastes), and consumer use of organic chemical-containing products including herbicides and pesticides. Concentrates

from Cincinnati, Philadelphia and New Orleans contained the highest levels of these substances.

- All DW concentrates contained halogenated species which probably originated from the chlorination of naturally occurring organic material in the source water. This result was the most pronounced for the Seattle and Miami concentrates.
- A tentative conclusion that the reverse osmosis membranes used for pre-concentration did not effectively retain (or, perhaps, absorbed) highly apolar species was based on a comparison of the RO-produced concentrates from a Cincinnati sampling with the concentrate produced by direct XAD-2 adsorption/elution prepared from the same volume of identical water. Based on the limited evidence, RO was more effective for recovering highly polar, water soluble materials, especially humic material.

The central conclusion to be made concerning the AWT concentrate analysis results was that the use of contact with granular activated carbon (GAC) in these plants was obviously effective in reducing the amount of organic material recoverable in the final concentrate. Almost without exception, the AWT concentrates contained less organic material in the analyzed fractions and resulted in fewer identified compounds and lower detected levels than the DW concentrates. For some of the AWT concentrates, these comparative differences were substantial. However, the sampled finished AWT water contained higher total organic carbon (TOC) levels than the sampled finished DW and, therefore, the conclusion is that the finished AWT water contained higher levels of material not recoverable by RO and/or not suitable for GC-MS analysis than did the finished DW. Assuming that the AWT influent contained organic material suitable for GC-MS analysis at levels at least as high as those for the finished DW, one must conclude that the GAC contact step in the AWT process was effective in reducing the levels of GC-MS analyzable organic substances to below those for the sampled DW. Compared to the DW concentrates, the AWT concentrates contained higher levels of fatty and other acids, phthalates, and poly glycol ethers (relatively polar species) but generally lower levels of apolar species attributable to the use or production of industrial organic chemicals. This observation supports the conclusion, above, concerning the effectiveness of GAC contact stages in the AWT plants. Higher efficiency for removing the apolar species (which are more suitable for GC-MS analysis) than the polar, more highly water soluble species is consistent with chemical expectations. One AWT plant (Escondido, California) employed RO rather than GAC contactor treatment. Since the Escondido concentrate contained less organic material and fewer species identifiable by GC-MS, the tentative conclusion is that RO is highly effective for final treatment for AWT systems. However, insufficient data are available to compare RO effectiveness to GAC treatment.

SECTION 3

RECOMMENDATIONS

Future work in attempting to correlate potential health effects of organic contamination in DW and AWT water with the nature of the organic materials present should employ biological testing of individual chemical group fractions of the organic concentrates rather than bulk concentrates. Such a strategy could greatly reduce the amount of chemical analysis required. Results from the DW concentrates indicated that more than 80 percent of the organic material present was humic material which was not suitable for characterization by GC-MS yet these materials may be responsible for a significant amount of biological activity. Standard methods are available for isolating the humic materials in concentrates. Separate biological testing of a humic/fulvic acid fraction as well as the fractions isolated for GC-MS analysis would greatly simplify the task of attempting to correlate the organic compounds present in the concentrate with the biological testing results. For example, the polar neutral fraction always contained a plethora of alcohols, ketones, diester plasticizers and mixed functionality species many of which are difficult to identify by GC-MS analysis. Certainly, many of these compounds are biologically inactive, and if this polar fraction consistently failed to show biological activity, GC-MS analysis could be omitted. The opposite case may be true for the aromatic fraction which represented only 0.05 to 1.0 percent of organic material in the concentrate.

Comparison of analysis results for concentrates prepared from identical DW samples by the RO-based method and by the direct XAD-2 adsorption/elution method suggested that much and possibly most of the apolar anthropogenic species present in the sampled water were not recovered by RO. These anthropogenic species are of the highest interest group for potential health effect investigation. On the other hand, direct XAD-2 adsorption/elution did not recover ionized, highly polar and macromolecular species such as humic/fulvic acids and poly glycols as well as the method employing RO pre-concentration. Development of a combination of these two methods could provide a concentrate more representative of the organic material present in the original water so that more reliable health effect conclusions could be made.

The compound identification results represented in this work constitute the most detailed chemical characterization of a wide variety of clean waters such as DW and finished AWT water from various sources. However, the results also show that only a small fraction of the organic material recovered into the concentrate is suitable for characterization by GC-MS methods. Detailed characterization of the major part of the organic material which was not suitable for direct GC-MS analysis should be performed to complete this work.

While these incomplete aspects have high importance for the health effects evaluation goal, their intrinsic scientific value alone justifies a continuation of the present work.

In future analytical work of this type, some minor modifications to the analytical scheme requiring further method development work can provide a more cost effective analysis:

- The use of polar capillary GC columns that are capable of higher temperature limits could eliminate the necessity for analyzing the high polarity, medium polarity and acid fractions on the apolar phase

- GC-MS analysis of the aromatic fraction should be restricted to the apolar GC column

- Based on the compound identification results of this study, additional compounds could be selected for computerized data searching. These compounds could be selected to profile different characteristics of source waters.

SECTION 4

BACKGROUND INFORMATION ON THE ORGANIC CONCENTRATES

CONCENTRATE PRODUCTION METHODS

Although none of the organic concentrates were produced by Battelle under the subject contract, some discussion of the concentrate production methodology is necessary to provide context to the discussions that follow.

All but four of the 36 DW and AWT concentrates were produced by Gulf South Research Institute (GSRI) under contracts 68-02-2090 (AWT) and 68-03-2367 (DW). The remaining four concentrates were produced in the EPA HERL-CI laboratory. Two of these four concentrates were produced by reverse osmosis (RO) procedures corresponding to those used by GSRI. The remaining concentrates (of which one was a process blank) were produced by direct XAD-2 adsorption with diethyl ether elution. In producing these concentrates at HERL-CI, half of a split stream was used to fill the reservoirs for RO processing while the other half was acidified to pH 2 in the flowing stream and passed directly over a column of XAD-2 resin. Elution of the XAD-2 resin with diethyl ether and subsequent concentration yielded the Cincinnati I XAD/DIRECT concentrate, code T1Y (the XAD-2 process blank was coded T2B), and RO processing of the other half of the sample provided the other two concentrates (coded T1C and T1X) by a procedure adapted from that used by GSRI, below (see Appendix E). Tables 1 and 2 list the DW and AWT samples, respectively, and also details concerning the sampling, source water and treatment plant.

The RO concentrate production methodology has been reported previously (1,2) and is only briefly summarized here. A schematic diagram of the RO processing unit is shown in Figure 1 (2). Sample water was processed batchwise at pH 5.5 through a cellulose acetate membrane. The permeate water was processed after pH adjustment to 10.0 through a second RO unit equipped with a DuPont Permasep® nylon fiber cartridge. The separate RO brines were recycled (with all cellulose acetate permeate being used as Permasep® feed) until the brine volumes were reduced to about 38 liters, or until salt precipitation became a problem. The two RO brines were sequentially extracted with pentane and methylene chloride. After acidification the extraction with methylene choride was repeated. Thus, after solvent evaporation, six separate organic extracts were obtained. For some samples, including all of the DW samples, the six solvent extracts were combined and analyzed as a composite concentrate. For some of the AWT samples, one or more of the six individual solvent extracts was selected for analysis individually (see Table 2).

The extraction of organic compounds from the RO brine was carried one step

TABLE 1. SOURCE WATER, SAMPLING AND CONCENTRATE PRODUCTION INFORMATION FOR DRINKING WATER CONCENTRATES

City	Date Sampled	Volume Sampled (liters)	Water Source (description; sampling location)	TOC[a] (mg/l)	Concentrates Analyzed	
					Code Name[b]	Method of Production[c,d]
Cincinnati, OH	10-17-78	1,460	Ohio River (containing contributions from industrial, chemical, agricultural and treated and untreated sewage; tap water, EPA Laboratories at 26 W. St. Clair Street)	not determined	T1C T1X T1Y	Solvent Extract XAD-2 Extract Direct XAD-2 Extraction/ diethyl ether elution (no RO processing)
Cincinnati, OH	01-14-80	7,110	Ohio River (as above; Kellogg Ave. Treatment Plant)	1.9	T4C T4X	Solvent Extract XAD-2 Extract
Miami, FL	02-03-76	2,270	Shallow Well (swamp-fed aquifers vulnerable to waste-disposal contamination; Preston Water Works)	6.4 ± 1	M2C M2X	Solvent Extract XAD-2 Extract
New Orleans, LA	01-14-76	6,620	Mississippi River (as above, for Ohio River, but more predominantly agricultural run-off; tap water, GSRI Laboratories)	1.7 ± 1	N2C N2X	Solvent Extract XAD-2 Extract
Ottumwa, IA	09-10-76	5,450	Des Moines River (predominantly agricultural run-off; Ottumwa Water Works)	2.4 ± 1	O2C O2X	Solvent Extract XAD-2 Extract
Philadelphia, PA	02-10-76	5,810	Delaware River (as above, for Ohio River, but more predominantly vulnerable to chemical and industrial pollution; Torresdale Water Works)	1.7 ± 1	P2C P2X	Solvent Extract XAD-2 Extract
Poplarville, MS	03-02-79	15,100	Deep Well (virtually organic-free; Poplarville Water Works)		V1C V1X	Solvent Extract XAD-2 Extract
Seattle, WA	11-05-76	11,750	Pristine Mountain Stream (essentially free of all organic pollutants except those from natural sources; Distribution System at 2700 Airport Way(Cedar River))	1.0 ± 1	S2C S2X	Solvent Extract XAD-2 Extract

a) determined by GSRI under EPA Contract 68-03-2367
b) the three digit code is used in the computer-printed tabulations
c) concentrates T1C, T1X and T1Y were produced by HERL-CI. The other concentrates were produced by GSRI under Contract 68-03-2367.
d) "Solvent extract" denotes a combination of the six solvent extracts of the cellulose acetate and nylon membrane RO brines produced from the sampled water. "XAD-2 extract" denotes a subsequent extraction of these two RO brines using XAD-2 resin with ethanol elution.

TABLE 2. SOURCE WATER, SAMPLING AND CONCENTRATE PRODUCTION INFORMATION FOR ADVANCED WASTE TREATMENT CONCENTRATES

Treatment Plant	Date Sampled	Influent Characteristics[a]	Water Treatment Sequence[a]	Finished Water Characteristics[a] TOC[b] (mg/1)	Disolved Solids (mg/1)	Concentrates Analyzed Code Name[c]	Method of Production (RO Brine Extraction)[d,e]
Blue Plains Washington, D.C.	09-19-74	essentially 100% municipal (domestic, weak strength; little industrial waste)	low lime clarification; breakpoint chlorination and neutralization (in parallel); GAC adsorption; dual media filtration	11.3	544	B1M B1N	CA CH_2Cl_2 CA Acidic CH_2Cl_2
Blue Plains Washington, D.C.	05-29-75	(as above)	low lime clarification; activated sludge nitrification; GAC adsorption; dual media filtration; chlorination	2 (8.8	na[f] 339)[g]	B2C	Combined
Dallas, TX	12-10-74	88% municipal by volume; 35% BOD, industrial and commercial; medium strength	primary clarification; activated sludge; secondary clarification; high lime clarification, recarbonation; mixed media filtration; GAC adsorption; chlorination	na (7.6	515 468)[g]	D2N	CA Acidic CH_2Cl_2
Escondido, CA	07-08-75	86% domestic, 14% industrial (large electronics industry component)	biological treatment by contact stabilization; mixed media filtration; reverse osmosis (75% permeation)	6.9	82	E1C	Combined
Lake Tahoe, CA	10-24-74	essentially 100% domestic of relatively low strength	primary coagulation; activated sludge and sedimentation; high lime coagulation and clairification; ammonia stripping; recarbonation; filtration; GAC adsorption; chlorination	na (10	na 387)[g]	L2P L2M L2N L2D	CA Pentane CA CH_2Cl_2 CA CH_2Cl_2 NYL Acidic CH_2Cl_2
Orange County, CA	01-27-76	30% industrial (predominantly pretreated metal plating and refining)	(main plant: primary clarification and trickling filtration) lime coagulation; ammonia stripping; two-stage recarbonation; mixed media filtration; GAC adsorption; chlorination	na (6.4	na 952)[g]	R1C	Combined
Orange County, CA	02-03-76	(as above)	(as above)	(as above)		R2C	Combined
Pomona, CA	09-25-74	90% municipal by volume; diverse industrial sources including some paper product waste	(main plant: primary sedimentation, activated sludge, final clarification) GAC adsorption; chlorination (1.5 hrs. contact with 10 mg/1 Cl_2 residual); GAC adsorption	na (11.0	496 511)[g]	C1P C1M C1N	CA Pentane CA CH_2Cl_2 CA Acidic CH_2Cl_2
Pomona, CA	10-02-74	(as above)	(as above, but without final GAC adsorption)	35.1 (12±11	434 517)[g]	C2N	CA Acidic CH_2Cl_2
Pomona, CA	06-17-75	(as above)	(as above for 09-25-74 but ozonation at 30 mg/1 and 21 min. contact time instead of chlorination)	na (12±8	na 571)[g]	C3C	Combined

a) Taken from reference 2.
b) TOC: total organic carbon.
c) The three digit code is used in the computer-printed tabulations.
d) Concentrates produced by GSRI under contract 68-03-2090 by methods report in reference 2 and summarized here in Section 4.A.
e) "CA" designates an RO brine produced by the cellulose acetate membrane; "NYL" designates an RO brine produced by the Permasep® nylon fiber RO unit; "Combined" designates a combination of all six RO extracts, see Section 4.A.
f) Information is not available.
g) Data averaged over the following number of determinations on different days; Blue Plains, 6; Dallas, 8; Lake Tahoe, 13; Orange County, 6; Pomona (all samplings), 9.

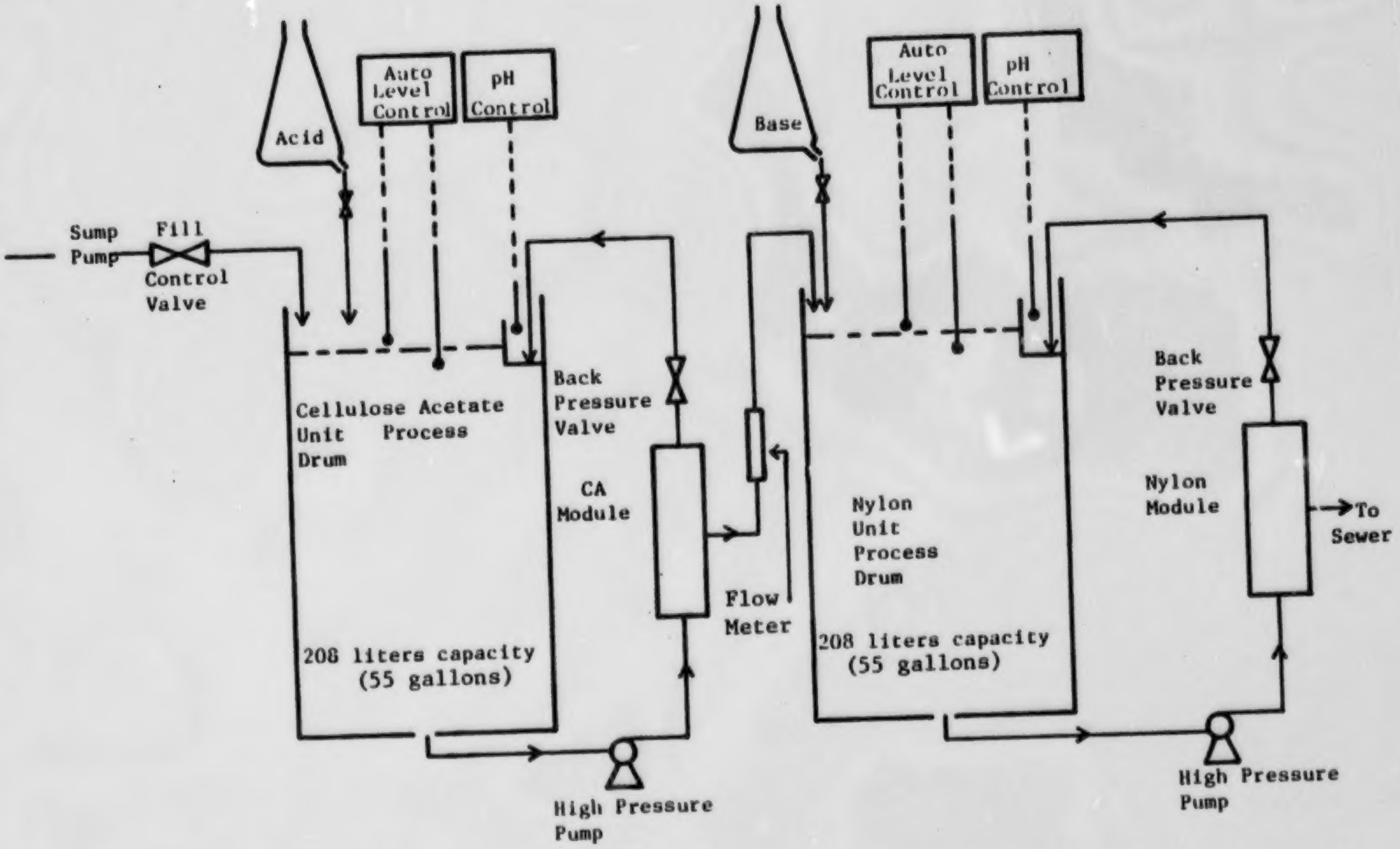
Sump
Pump
Fill
Control
Valve
Acid
Auto
Level
Control
pH
Control
Cellulose Acetate
Unit Process
Drum
208 liters capacity
(55 gallons)
Back
Pressure
Valve
CA
Module
High Pressure
Pump
Flow
Meter
Base
Auto
Level
Control
pH
Control
Nylon
Unit
Process
Drum
208 liters capacity
(55 gallons)
Back
Pressure
Valve
Nylon
Module
To
Sewer
High Pressure
Pump

Figure 1. Schematic diagram of the reverse osmosis concentrator used by GSRI. (Taken from EPA publication 600/2-78-016, February, 1978; available through NTIS)

further for the DW concentrates. Following solvent extraction, the reverse osmosis brine was extracted with XAD-2 resin followed by ethanol elution to obtain an additional amount of organic material which was generally greater (on a residue weight basis) than that obtained from solvent extraction. Unfortunately, three of these XAD-2 concentrates were seriously contaminated with artifacts generally described as XAD "resin bleed", and the analysis results of these concentrates are less useful than those for the others. The XAD-2 artifact problem is addressed in Section 6, Results and Discussion of this report.

THE RO METHOD BLANK

The RO methodology for producing organic concentrates from large volumes of relatively clean water was an emerging technology when the concentrates were produced. Progress has been made since then to improve recovery and reduce artifact generation, and HERL-CI is currently sponsoring a program to characterize the performance of various organic concentration techniques from large volumes of clean water under carefully controlled conditions. As might be expected, obtaining an ideal RO process blank is very difficult. Previous attempts have shown that RO processing of very large volumes of high quality reagent water produced a concentrate that contained numerous compounds (1). Moreover, the use of reagent water is inappropriate since the lack of dissolved salts might be expected to modify the contribution of the RO apparatus to the blank. For this reason, the Poplarville, Mississippi, concentrate (see Table 1) was used as a blank. The Poplarville water originates from deep wells tapping an aquifer which is extraordinarily organic-free yet contains dissolved salts at normal levels. Over 15,000 liters of this water were used to prepare the Poplarville blank concentrate. This volume is greater than the AWT volumes by a factor of 10 and greater than the DW volumes by a factor of 1.4 to 10 (see Tables 1 and 2). In addition, the Poplarville concentrate represents true field sampling experimental conditions. Of more concern than the authenticity of the blank is the lack of knowledge of the efficiency of RO membrane retention of relatively small organic molecules under conditions of extremely low concentration and high volumes of processed water. This issue is addressed in Section 6, Results and Discussion.

In addition to the two Poplarville, Mississippi, RO process blank samples, three other blank concentrates were analyzed. The first blank corresponds to evaporated pentane and methylene chloride as a control for organic materials present in solvents used to extract the RO brine. This concentrate is designated by the code, X1C, in the tables of combined concentrate results (Tables 9 through 15). The second blank, designated X1X in the computer-printed tables, was generated from ethanol elution of XAD-2 resin. The third blank sample designated by the code, T2B,was also a solvent elution of XAD-2 resin, but in this case the solvent was diethyl ether. This blank sample was actually a process blank for one of the three concentrates produced by HERL-CI.

THE WATER USED FOR CONCENTRATE PRODUCTION

With the exception of the three concentrates produced by HERL-CI and the New Orleans sampling, all of the DW sampling was performed at municipal DW plants. The three HERL-CI produced concentrates and two New Orleans concentrates were generated from DW taken from the tap at the HERL-CI and GSRI laboratories, respectively. Some of the relevant information for the DW sites is given in Table 1. Similar information concerning the AWT concentrates produced by GSRI is given in Table 2.

The cities sampled for DW concentrates were chosen by EPA to provide a typical range in types of raw water and methods of treatment. Results of the analysis of volatile organics from DW sampled from these cities has previously been reported (3). Details concerning the DW treatment plants and the standard water quality parameters (TOC, pH, hardness) at the time of sampling are available from U.S. EPA/HERL in Cincinnati. Note that none of the DW concentrates were prepared from finished water treated by contact with activated carbon. In contrast, all but one of the AWT plants (Table 2) incorporated activated carbon contact as either the last step in the treatment scheme or the step preceding final chlorination. Detailed descriptions of each of the AWT plants sampled and pre-treatment and post-treatment data on suspended solids, BOD, COD, TOC, ammonia, pH, hardness, inorganic anions, and other standard water quality parameters have been reported previously (2).

SECTION 5

ANALYTICAL SCHEME

RATIONALE FOR THE ANALYTICAL SCHEME

The analytical scheme described below was developed during the first year of the contract through the joint efforts of Battelle researchers and the EPA Project Officer.

The concentrate samples processed through the analytical scheme were extremely complex organic mixtures in about 1 to 2 ml of solvent. To illustrate this complexity, a partial chromatogram from glass capillary GC analysis of the unpartitioned Pomona II acidified methylene chloride concentrate is shown in Figure 2. A 30 meter (0.26 mm I.D.) SP2100 coated glass capillary column with relatively high efficiency was used to produce this chromatogram. The column used had a separation number of 36 between the C_{13} and C_{14} hydrocarbons of the test mixture. In the partial chromatogram of Figure 2, over 200 resolved and partially resolved GC peaks were obtained between 60°C and 150°C. The baseline rise between 130°C and 210°C is due to mixture component co-elution rather than detector drift. Identification of a significant number of the multitude of species in Figure 2 would be difficult even with glass capillary GC-MS. The analytical scheme shown in Figure 3 was specifically designed to enable the identification of a maximum number of the organic species present in these complex organic mixtures.

The analytical scheme includes addition of deuterated internal standards to the concentrate, fractionation of the concentrate through a combination of extraction under both acidic and basic conditions, partitioning of neutral compounds on a short silica gel column, and, analysis of the partitioned fractions as well as the unpartitioned concentrate by glass capillary GC-MS. Analysis of the unpartitioned concentrate was omitted for the DW concentrates produced by XAD-2 extraction of RO brine. The GC-MS analyses were conducted on two types of wall-coated open-tubular glass capillary GC columns, one containing a non-polar liquid phase SP2100) and the other a polar liquid phase (SP1000).

Process blank samples were produced simultaneously during concentrate partitioning. Also, the performance of each analytical instrument was monitored daily to ensure the reliability of the analytical data.

Each aspect of the analytical scheme is described in detail in the sections that follow. Quality control features are described in the context of this section and are not presented separately.

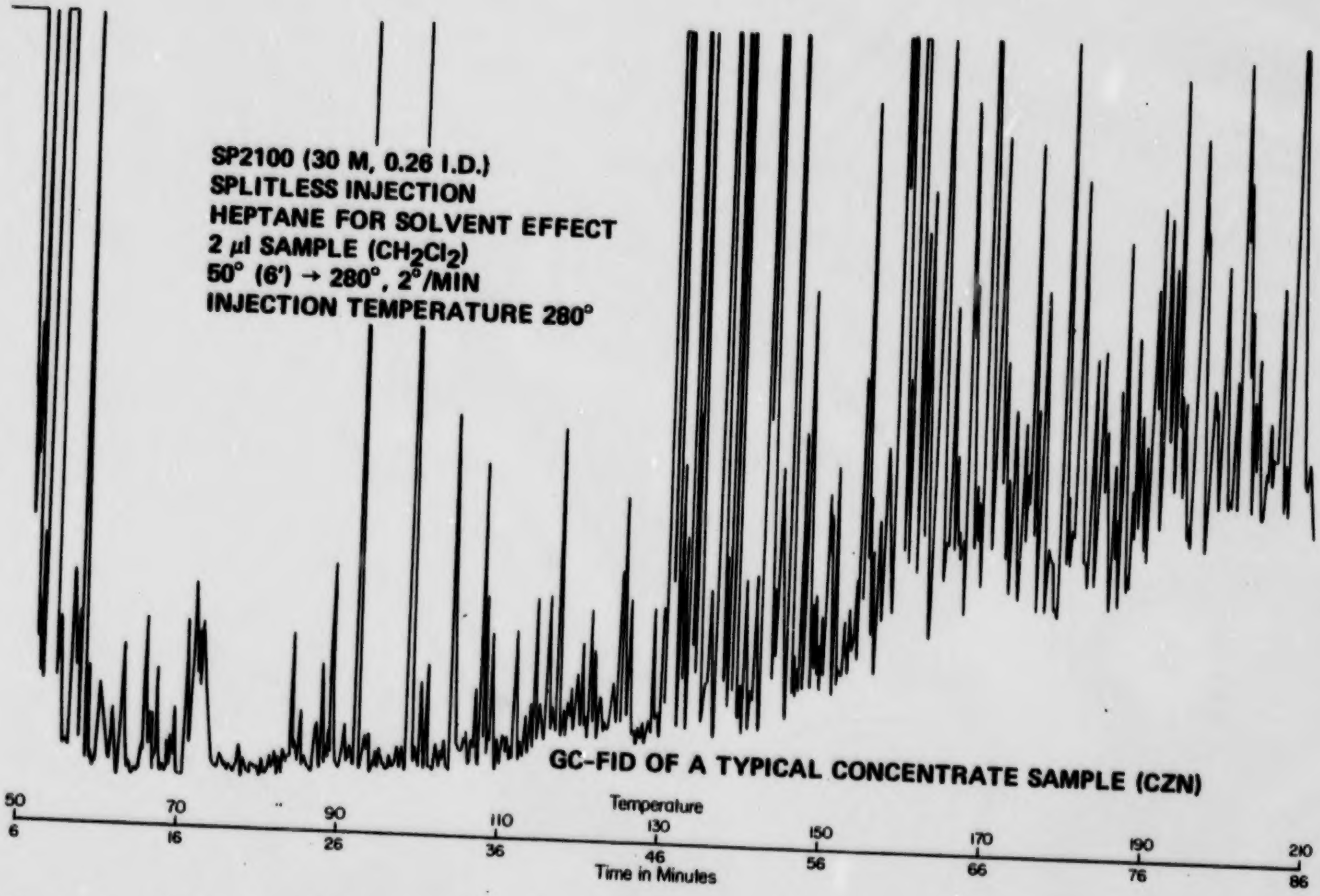

Figure 2. Partial gas chromatogram (FID) of a typical unpartitioned water concentrate sample.

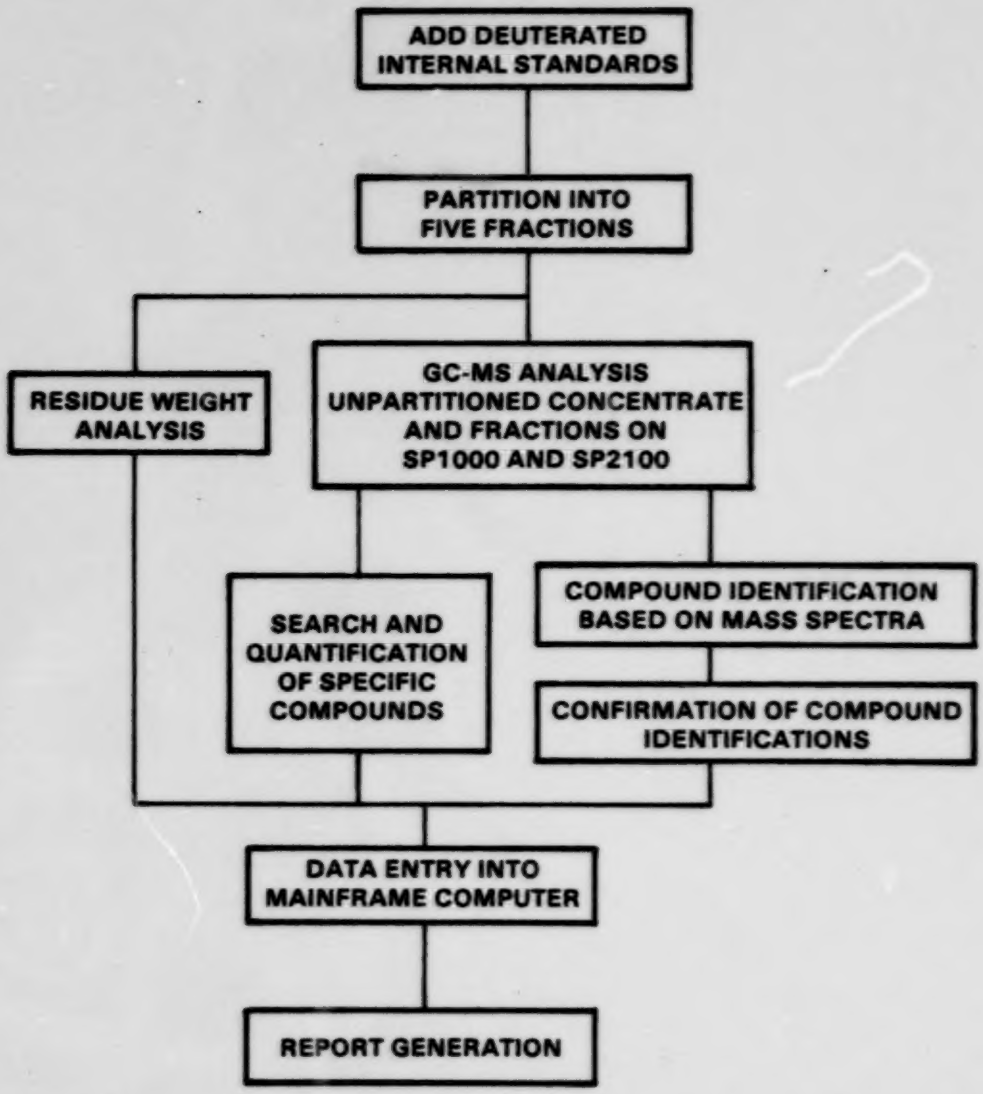
ADD DEUTERATED INTERNAL STANDARDS
PARTITION INTO FIVE FRACTIONS
RESIDUE WEIGHT ANALYSIS
GC-MS ANALYSIS UNPARTITIONED CONCENTRATE AND FRACTIONS ON SP1000 AND SP2100
SEARCH AND QUANTIFICATION OF SPECIFIC COMPOUNDS
COMPOUND IDENTIFICATION BASED ON MASS SPECTRA
CONFIRMATION OF COMPOUND IDENTIFICATIONS
DATA ENTRY INTO MAINFRAME COMPUTER
REPORT GENERATION

Figure 3. Analytical scheme for the analysis of water concentrates.

INTERNAL STANDARDS

Thirteen deuterium-labeled compounds (Table 3) were added to the concentrate before partitioning to serve as internal standards. In addition, hexaethylbenzene was added to each fraction prior to analysis by GC-MS. These internal standards served three purposes:

1. Monitoring fractionation recoveries. The deuterium-labeled internal standards were selected so that at least one compound was partitioned into each fraction (Table 3). Recoveries of internal standards in the various fractions could be determined from the GC-MS data with any significant departure from the normal recoveries indicating abnormal performance of the partitioning scheme.

2. Calculation of relative retention values. A relative retention value was calculated for each GC peak by dividing the absolute retention time by that of the internal standard, hexaethylbenzene. Relative retention values were required for confirmation of tentative identifications of compounds based on mass spectra.

3. Quantification. The amounts of specific search compounds found in the unpartitioned concentrate and the partitioned fractions were calculated from GC peak areas in the extracted ion current profile (EICP) chromatogram relative to those of appropriate deuterated internal standards. In addition, comparison of the size of the hexaethylbenzene GC peak to those of the identified components was used to provide a less accurate but more easily accomplished quantitative estimation for every identified component.

PARTITIONING OF THE CONCENTRATES

The partitioning scheme was designed to separate the complex concentrates into acidic, basic, and neutral compounds by aqueous/organic liquid-liquid partitioning. The neutral compounds were further partitioned with silica gel chromatography. The scheme is a modification of the procedure reported by Ishiwatari and Hanya (4). Not only does the scheme separate the concentrate into fractions more suitable for GC-MS analysis, it also isolates the organic acids and phenols into a fraction which can be conveniently converted into methyl esters or ethers by treatment with diazomethane. The methylated acids and phenols exhibit better chromatographic properties than the corresponding free acid compounds.

A schematic representation of the originally developed partitioning procedure for concentrates produced by solvent extraction of RO brine is shown in Figure 4. A modified procedure for partitioning the concentrates produced by XAD-2 resin extraction of the DW RO brines is shown in Figure 5. Modification of the original scheme was necessary for these samples because of the extremely high level of acidic material (apparently humic substances) which made the original extraction of the bases with small volumes of 5% H_2SO_4 (as

TABLE 3. DEUTERIUM-LABELED COMPOUNDS USED AS INTERNAL STANDARDS

Compound	Fractions in Which Compound is Recovered[a]
Pyridine-D_5	Combined[b]
Aniline-D_5	Combined
Benzoic acid-D_5	Derivatized Acids
Phenol-D_5	Derivatized Acids
Eicosane-D_{42}	Aliphatic Hydrocarbons[c]
Bromobenzene-D_5	Aromatic
1,4-Dibromobenzene-D_4	Aromatic
Naphthalene-D_8	Aromatic
Chrysene-D_{12}	Aromatic
Perylene-D_{12}	Aromatic
Nitrobenzene-D_5	Aromatic and Combined[b]
Nitronaphthalene-D_7	Aromatic and Combined[b]
Dimethylterephthalate-D_4	High Polarity

a) See Figures 4 and 5 for production details of the analyzed fractions.

b) Extracted bases combined with medium polarity neutrals.

c) This fraction is not analyzed by GC-MS.

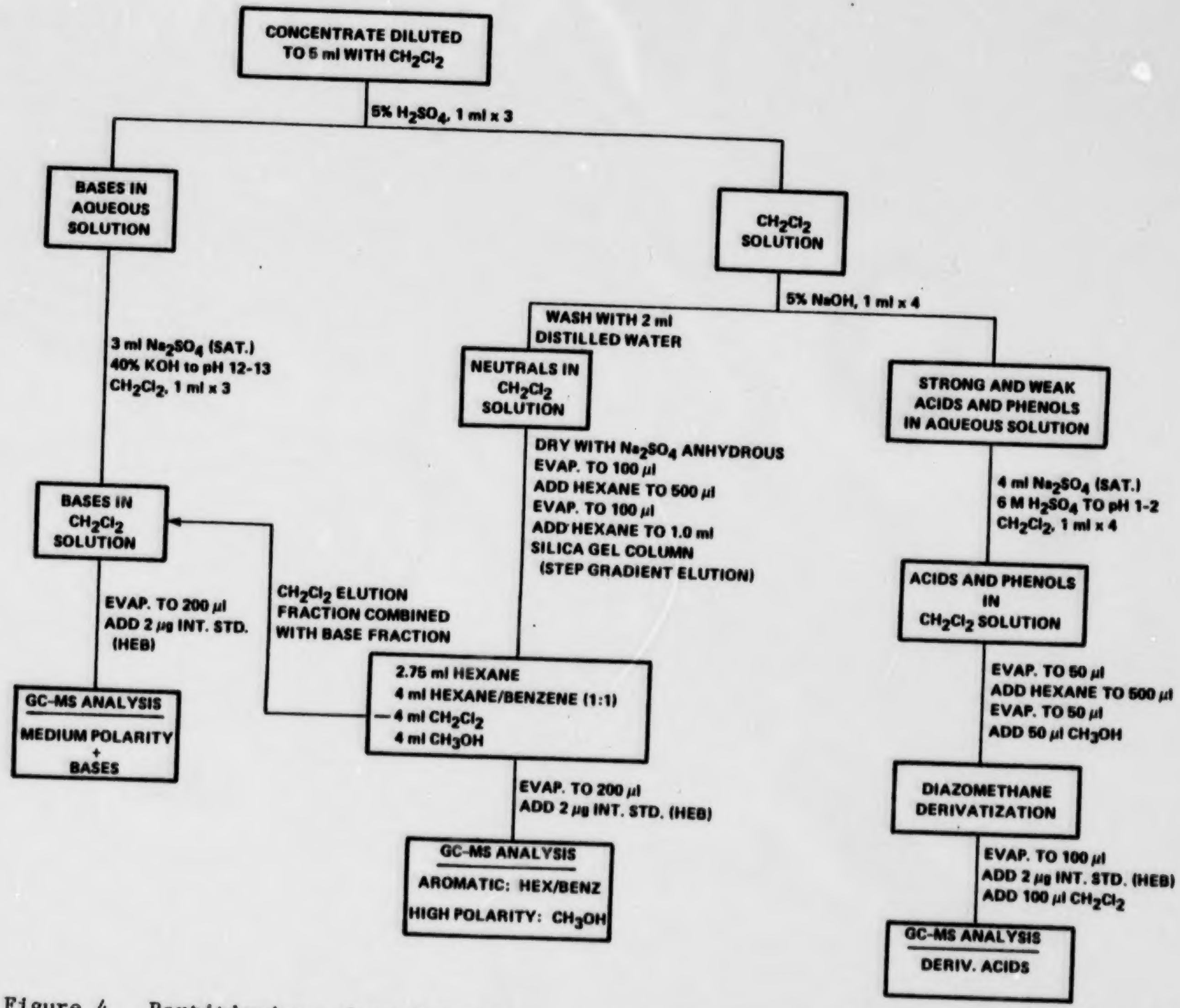
CONCENTRATE DILUTED TO 5 ml WITH CH_2Cl_2
5% H_2SO_4, 1 ml x 3
BASES IN AQUEOUS SOLUTION
CH_2Cl_2 SOLUTION
5% NaOH, 1 ml x 4
WASH WITH 2 ml DISTILLED WATER
3 ml Na_2SO_4 (SAT.)
40% KOH to pH 12-13
CH_2Cl_2, 1 ml x 3
NEUTRALS IN CH_2Cl_2 SOLUTION
STRONG AND WEAK ACIDS AND PHENOLS IN AQUEOUS SOLUTION
DRY WITH Na_2SO_4 ANHYDROUS
EVAP. TO 100 µl
ADD HEXANE TO 500 µl
EVAP. TO 100 µl
ADD HEXANE TO 1.0 ml
SILICA GEL COLUMN
(STEP GRADIENT ELUTION)
4 ml Na_2SO_4 (SAT.)
6 M H_2SO_4 TO pH 1-2
CH_2Cl_2, 1 ml x 4
BASES IN CH_2Cl_2 SOLUTION
ACIDS AND PHENOLS IN CH_2Cl_2 SOLUTION
EVAP. TO 200 µl
ADD 2 µg INT. STD.
(HEB)
CH_2Cl_2 ELUTION FRACTION COMBINED WITH BASE FRACTION
2.75 ml HEXANE
4 ml HEXANE/BENZENE (1:1)
4 ml CH_2Cl_2
4 ml CH_3OH
EVAP. TO 50 µl
ADD HEXANE TO 500 µl
EVAP. TO 50 µl
ADD 50 µl CH_3OH
GC-MS ANALYSIS
MEDIUM POLARITY + BASES
EVAP. TO 200 µl
ADD 2 µg INT. STD. (HEB)
DIAZOMETHANE DERIVATIZATION
GC-MS ANALYSIS
AROMATIC: HEX/BENZ
HIGH POLARITY: CH_3OH
EVAP. TO 100 µl
ADD 2 µg INT. STD. (HEB)
ADD 100 µl CH_2Cl_2
GC-MS ANALYSIS
DERIV. ACIDS

Figure 4. Partitioning scheme for water concentrates derived from solvent extraction of reverse osmosis concentrates.

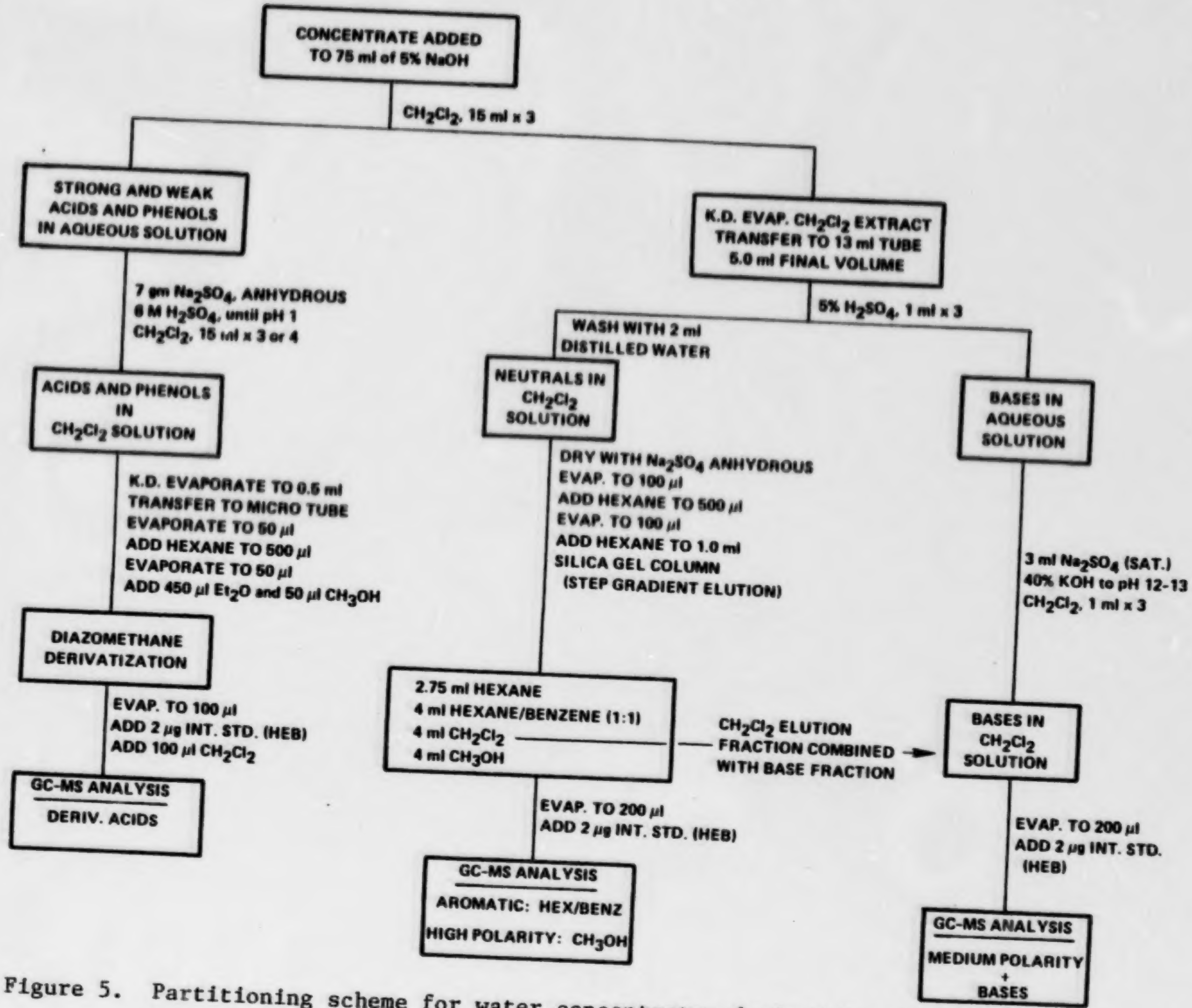
CONCENTRATE ADDED TO 75 ml of 5% NaOH
CH_2Cl_2, 15 ml x 3
STRONG AND WEAK ACIDS AND PHENOLS IN AQUEOUS SOLUTION
K.D. EVAP. CH_2Cl_2 EXTRACT TRANSFER TO 13 ml TUBE 5.0 ml FINAL VOLUME
7 gm Na_2SO_4, ANHYDROUS
6 M H_2SO_4, until pH 1
CH_2Cl_2, 15 ml x 3 or 4
5% H_2SO_4, 1 ml x 3
WASH WITH 2 ml DISTILLED WATER
ACIDS AND PHENOLS IN CH_2Cl_2 SOLUTION
NEUTRALS IN CH_2Cl_2 SOLUTION
BASES IN AQUEOUS SOLUTION
K.D. EVAPORATE TO 0.5 ml
TRANSFER TO MICRO TUBE
EVAPORATE TO 50 µl
ADD HEXANE TO 500 µl
EVAPORATE TO 50 µl
ADD 450 µl Et_2O and 50 µl CH_3OH
DRY WITH Na_2SO_4 ANHYDROUS
EVAP. TO 100 µl
ADD HEXANE TO 500 µl
EVAP. TO 100 µl
ADD HEXANE TO 1.0 ml
SILICA GEL COLUMN
(STEP GRADIENT ELUTION)
3 ml Na_2SO_4 (SAT.)
40% KOH to pH 12-13
CH_2Cl_2, 1 ml x 3
DIAZOMETHANE DERIVATIZATION
2.75 ml HEXANE
4 ml HEXANE/BENZENE (1:1)
4 ml CH_2Cl_2
4 ml CH_3OH
CH_2Cl_2 ELUTION FRACTION COMBINED WITH BASE FRACTION
BASES IN CH_2Cl_2 SOLUTION
EVAP. TO 100 µl
ADD 2 µg INT. STD. (HEB)
ADD 100 µl CH_2Cl_2
EVAP. TO 200 µl
ADD 2 µg INT. STD. (HEB)
EVAP. TO 200 µl
ADD 2 µg INT. STD. (HEB)
GC-MS ANALYSIS
DERIV. ACIDS
GC-MS ANALYSIS
AROMATIC: HEX/BENZ
HIGH POLARITY: CH_3OH
GC-MS ANALYSIS
MEDIUM POLARITY + BASES

Figure 5. Partitioning scheme for water concentrates derived from XAD-2 extraction of reverse osmosis concentrates.

in Figure 4) impossible. These two partitioning schemes yield fractions which are essentially equivalent.

In partitioning the solvent extract concentrates (Figure 4), the bases were first extracted from the concentrate with 5% H_2SO_4. After adjusting the solution to pH 12-13, the bases were back-extracted into methylene chloride. The volume of the methylene chloride solution of the bases was then reduced to about 500 µl. Since this fraction containing extracted bases was usually not very complex, it was combined with another fraction from the silica gel chromatography of the neutrals, the methylene chloride fraction, which also was generally less complex than other analyzed fractions. This combined fraction was reduced to about 200 µl and 2.0 µg of the internal standard, hexaethylbenzene (HEB), was added. Analysis of these two fractions as a combined fraction resulted in a significant savings in time with virtually no loss of compound identification capability.

The acidic and phenolic compounds were extracted from the methylene chloride solution with 5% NaOH. In the case of XAD-type drinking water concentrates (Figure 5), the partitioning of the acids into 5% NaOH preceded the base extraction step above, and was done on a much larger scale to accommodate the relatively high concentration of extractable acidic material. The remaining base/neutral fraction was reduced in volume to allow proceeding on a scale similar to that of Figure 4. The extracted acids were back-extracted with methylene chloride after acidification to pH 1 to 2 and addition of Na_2SO_4. Prior to derivatization with diazomethane, the methylene chloride solvent was removed by solvent exchange to hexane. Without the solvent exchange, the diazomethane was found to react with the methylene chloride to generate a homologous series of chlorinated hydrocarbons which unacceptably complicated identification of the methylated acids and phenols.

The neutral compounds remaining after removal of the acids and bases were further partitioned into four fractions using a modification of an accepted pesticide micro-column separation procedure (5,6) employing open-column chromatography on 5% deactivated silica gel (Woelm type 02747, 70-150 mesh). Three identical silica gel columns (∿0.55 x 7 cm in a 6-inch disposable Pasteur pipette with a glass wool plug in the bottom and 6 to 8 mm of anhydrous granular Na_2SO_4 at the top) were prepared in a paralled fashion. Two columns were used for preparation of the sample and process blank fractions. The third column was used only to check the accuracy of the silica gel deactivation which was indicated by the volume of hexane required to elute anthracene from the column. The anthracene elution volume was monitored visually by a UV lamp of long wavelength (366 nm). One hundred micrograms of anthracene in 30 µl of hexane was applied to the column. Using hexane as the elution solvent, correct deactivation of the silica gel (5% water, by weight) was indicated by anthracene elution beginning after 7 ±0.5 ml of hexane had passed through the column. For 7% and 3% deactivation the volume of hexane used to eluate anthracene was found to be 11 ±0.5 and 5.5 ±0.5 ml, respectively.

Four elution solvents were used to partition the neutral compounds on silica gel (Figures 4 and 5). These solvents were applied to the column in the following sequence: 2.75 ml of hexane, 4 ml of hexane/benzene (1:1), 4 ml of methylene chloride, and 4 ml of methanol. After elution, the first 2.75 ml of hexane contained mostly alkanes and alkenes and only a small proportion of other compounds of interest, such as hexachlorobenzene. Since alkanes and alkenes are not considered potentially hazardous chemicals, this aliphatic hydrocarbon fraction was not analyzed except for the determination of its residue weight.

All of the volume reductions except for one Kuderna-Danish (K-D) distillation shown in Figure 5 were performed using an N-EVAP® Analytical Concentrator, Model 111 (Organomation Associates, Northborough, Main). Sample volumes were reduced in 4.0 ml capacity Chromaflex® tubes (Kontes, Vineland, New Jersey) which were tightly capped with aluminum foil. Ultra-pure nitrogen (99.999%, Matheson) was introduced to the tube with a blunt 18 guage needle inserted to just below the foil cap. The N_2 flow was controlled at 1.5 to 2.5 ml/min while the bottom of the tube was immersed in a water bath maintained at the boiling point ($\pm$ 3°C) of the primary solvent consitituent of the sample. Under these conditions, very gentle, nearly unobservable solvent refluxing was maintained in the upper part of the tube during solvent evaporation. These very mild conditions allowed reduction of a 3.5 ml sample to about 200 μl in 6 to 14 hours, depending on the vapor pressures, heats of vaporization and boiling points of the solvent constituents. This sample evaporation was used at the direction of the Project Officer with very little modification or attempts at further recovery optimization. It should be noted that this extremely slow solvent evaporation does not correspond to the usually encountered procedure of solvent blow-down under N_2.

RESIDUE WEIGHT ANALYSIS

In order to determine the quantities or organic material partitioned into the fractions, an aliquot of each fraction and process blank was evaporated to constant weight on a 12 mm square of aluminum foil, and the residues were accurately weighed to the nearest 2 μg on a Mettler ME30 microbalance. Residue weights were also determined for the unpartitioned concentrates. A sufficient volume of sample was evaporated to result in a minimum of about 20 μg of residue although no more than one half of a given sample was consumed for this purpose. Generally, only the process blank aliquots evaporated to net weights of less than 20 μg.

GAS CHROMATOGRAPHIC ANALYSIS

The partitioned fractions were very complex and required the use of high resolution gas chromatography to resolve the individual components. Wall-coated open-tubular glass capillary GC columns were used for these analyses with two different liquid phases: SP1000 (polar) and SP2100 (non-polar). These two types of coatings effectively complemented each other so that compounds which co-eluted on one column were usually well-separated on the other column. Also, high boiling or high polarity compounds which did not elute from the polar column could be observed on the non-polar column. The columns used in the initial stages were purchased from the J & W Scientific Company. For the final year of GC-MS analysis activity, columns of both polarities were made at Battelle.

Before a capillary GC column was accepted for analytical use, it had to meet the following minimum performance requirements:

- For SP2100 columns (30 M, 0.25 mm I.D.) operated at 100°C with a helium carrier velocity of 23 cm/sec:

  (1) N_{eff}= 80,000 (C_{14}), minimum
  (2) SN = 35 (C_{13}-C_{14}), minimum
  (3) Decylaldehyde, no tailing
  (4) Decanol tailing: peak base = 4.00 times the peak base of C_{13}, miximum
  (5) Acid/base ratio: 2,6-dimethylphenol:2,4-dimethylaniline ratio of 0.5 to 2.0, peak height basis
  (6) Sample capacity: 50 ng of C_{14}, no fronting

- For SP1000 columns (40 M, 0.25 mm I.D.) operated at 125°C with a helium carrier flow velocity of 23 cm/sec:

  (1) N_{eff}= 100,000 (C_{18}), minimum
  (2) SN = 25 (C_{17}-C_{18}), minimum
  (3) Decylaldehyde, no tailing
  (4) Decanol, no tailing
  (5) Acid/base ratio: 0.5 to 2.0, as above
  (6) Sample capacity, 50 ng of C_{18}, no fronting

Examples of GC-FID chromatograms resulting from analysis of the GC test mixture on acceptable SP2100 and SP1000 glass capillary columns are shown in Figures 6 and 7, respectively.

In initial stages of the work, all partitioned fractions and corresponding blank samples as well as unpartitioned concentrates, were analyzed by GC-FID on both capillary column phases prior to analysis by GC-MS. This preliminary analysis provided both a screening function to assess the sensitivity that would be required for GC-MS analysis, and also a quality control measure to ensure that GC-MS chromatography was performing optimally and that there were not significant amounts of late-eluting material. As experience was gained with the samples and GC-MS performance aspects, this preliminary screening was no longer required and, thus, was performed only as necessary. The following chromatographic analysis conditions were used for both the GC-FID screening analyses and the GC-MS analyses:

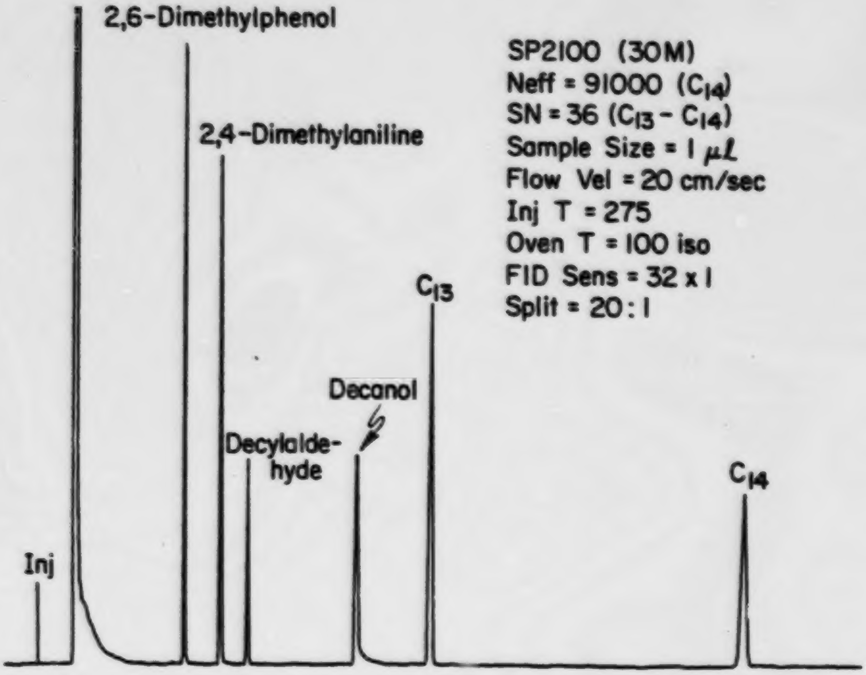

Figure 6. Typical column evaluation chromatogram for a 30M SP2100 (apolar) capillary column.

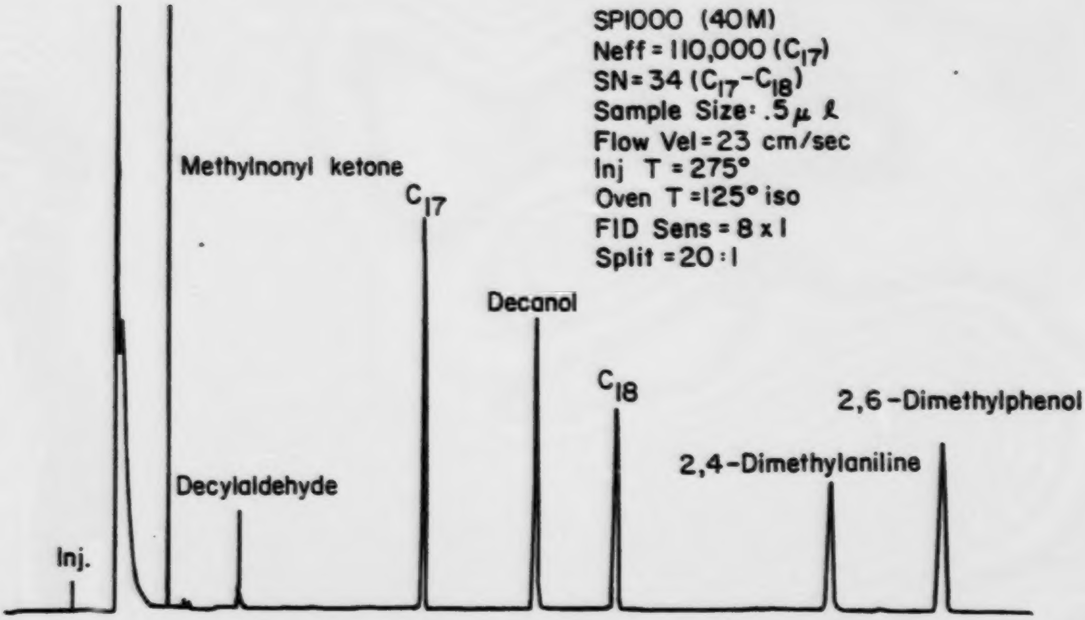

Figure 7. Typical column evaluation chromatogram for a 40M SP1000 (polar) capillary column.

GC-FID Operating Conditions

Instrument: Carlo Erba Model 2150

	SP1000 (40 M, 0.25 mm I.D.)	SP2100 (30 M, 0.25 mm I.D.)
Injector temperature	250°	275°
Initial column temperature (hold)	50°(6 min)	RT (3 min) 50°(3 min)
Program rate	2°/min	2°/min
Upper temperature limit	225°	280°
Injection volume (splitless)	2 µl sample plus 1 µl heptane	2 µl sample
Detector temperature	250°	275°
Helium flow velocity	23 to 25 cm/sec at 125°C	23 to 25 cm/sec at 100°C

GLASS CAPILLARY GC-MS ANALYSIS

Mass Spectrometer Performance Quality Assurance

GC-MS analysis of the partitioned fractions and the unpartitioned concentrates, as well as corresponding blank samples, provided the primary basis for identification and quantification of organic compounds in the concentrates. In order to ensure that all GC-MS data acquired were of high quality, the total GC-MS system performance was rigorously evaluated each day before undertaking analysis of concentrate samples. The GC-MS performance evaluation included the following operations:

(1) A check of the mass calibration by acquiring a spectrum of perfluorotributylamine (FC-43) using signal sampling at 0.1 amu intervals.

(2) An evaluation of the mass spectrometer resolution and mass discrimination by analysis of decafluorotriphenylphosphine (DFTPP) according to the recommendations of Eichelberger, Harris, and Budde (7).

(3) GC-MS analysis of a test mixture referred to as the Standard GC Separation Mixture (SGCSM). This mixture was designed to evaluate the following performance characteristics:

- Proper MS sensitivity, resolution, and high-mass/low-mass ion sensitivity ratio
- Proper functioning of the splitless injection system

- Adequate capillary GC column efficiency
- Suitable capillary GC column neutrality (neither acidic nor basic), and activity toward polar materials
- Absence of adsorptive sites or cold spots in the GC column and transfer line.

Typical GC-MS reconstructed gas chromatograms of the SGCSM test mixtures for the SP2100 and SP1000 columns are shown in Figures 8 and 9, respectively. The components of each mixture are labeled on the chromatogram. The mass spectrometer operating conditions and data acquisition parameters used for this test are identical to those used for sample analyses. The chromatographic conditions for the SGCSM test of both columns are as follows:

Sample:	5 ng/µl, each component in 90% n-decane
Injection:	2 µl; splitless
Carrier:	He at 23 cm/sec
Program:	140°C 3 min; 140 to 200° at 20°C/min; isothermal at 200°C
Data acquisition:	Start data acquisition at 8 min (SP2100) or 10 min (SP1000)

The chromatographic features which were monitored to detect degradation of the chromatographic and mass spectrometric systems are noted on the test chromatograms. Generally, failure of SP2100 columns was indicated by decanol tailing and acid-base ratio failure in advance of loss of coating efficiency while the opposite was true for the SP1000 column which was much more resistant to performance degradation.

Mass Spectrometer Operating Conditions

Instrument:	GC: Finnigan 9500 with a Grob-type split/splitless injector (identical to that of the Carlo Erba 2150 GC) and a direct introduction (no separator) transfer line (fused silica in final year of work only) MS: Finnigan 3200 Data System: Systems Industries System/150 with Battelle-modified software and equipped with a real-time clock.
Ionization:	70 eV electron impact at 150 to 350 µA total emission
Source Voltages:	Ion energy: 2 to 8 Volts (scan programmed) Extractor/repeller: 2 to 11 Volts Lens: ∿−80 Volts

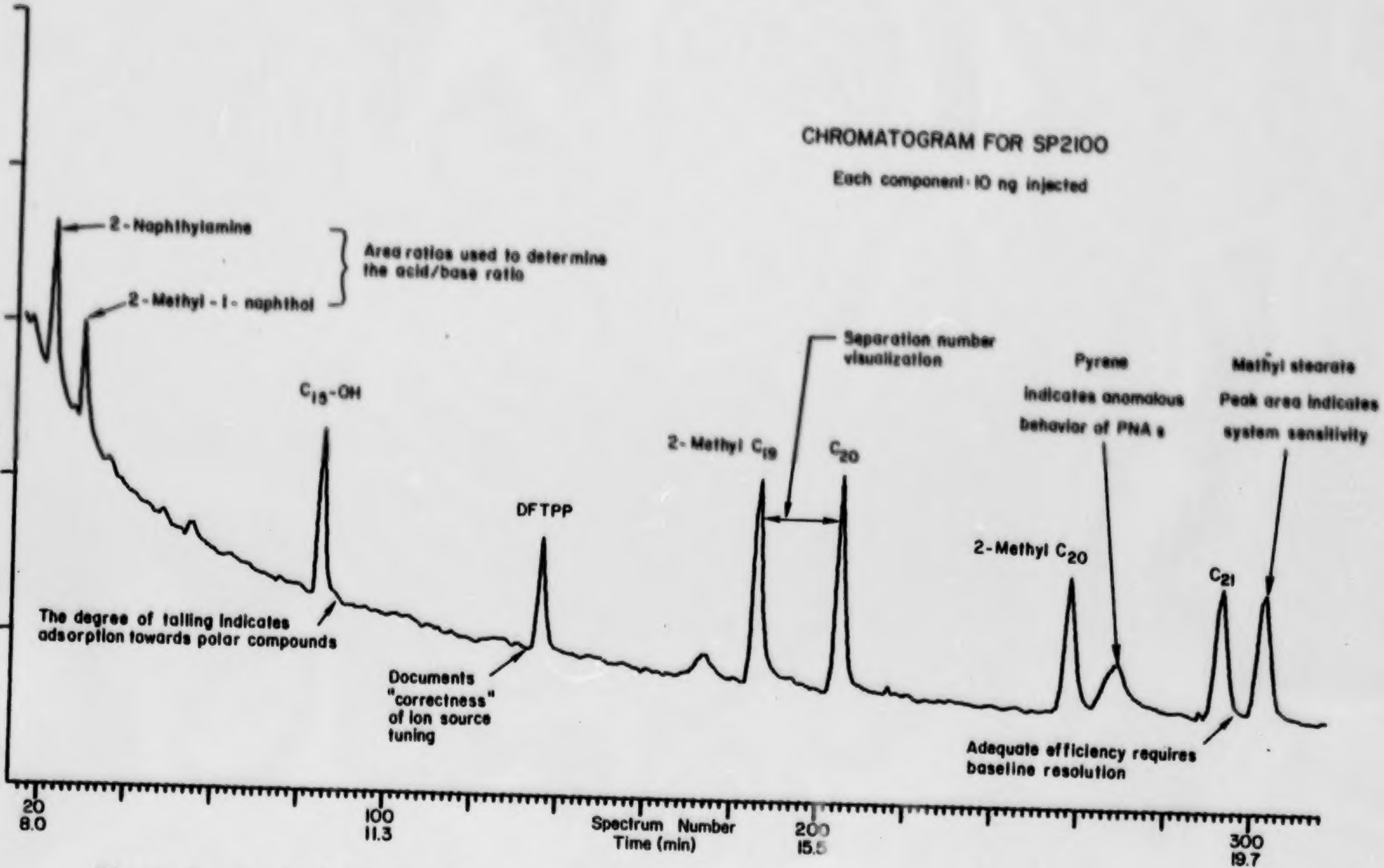

Figure 8. Typical GC-MS daily performance verification test chromatogram for the SP2100 (apolar) capillary column.

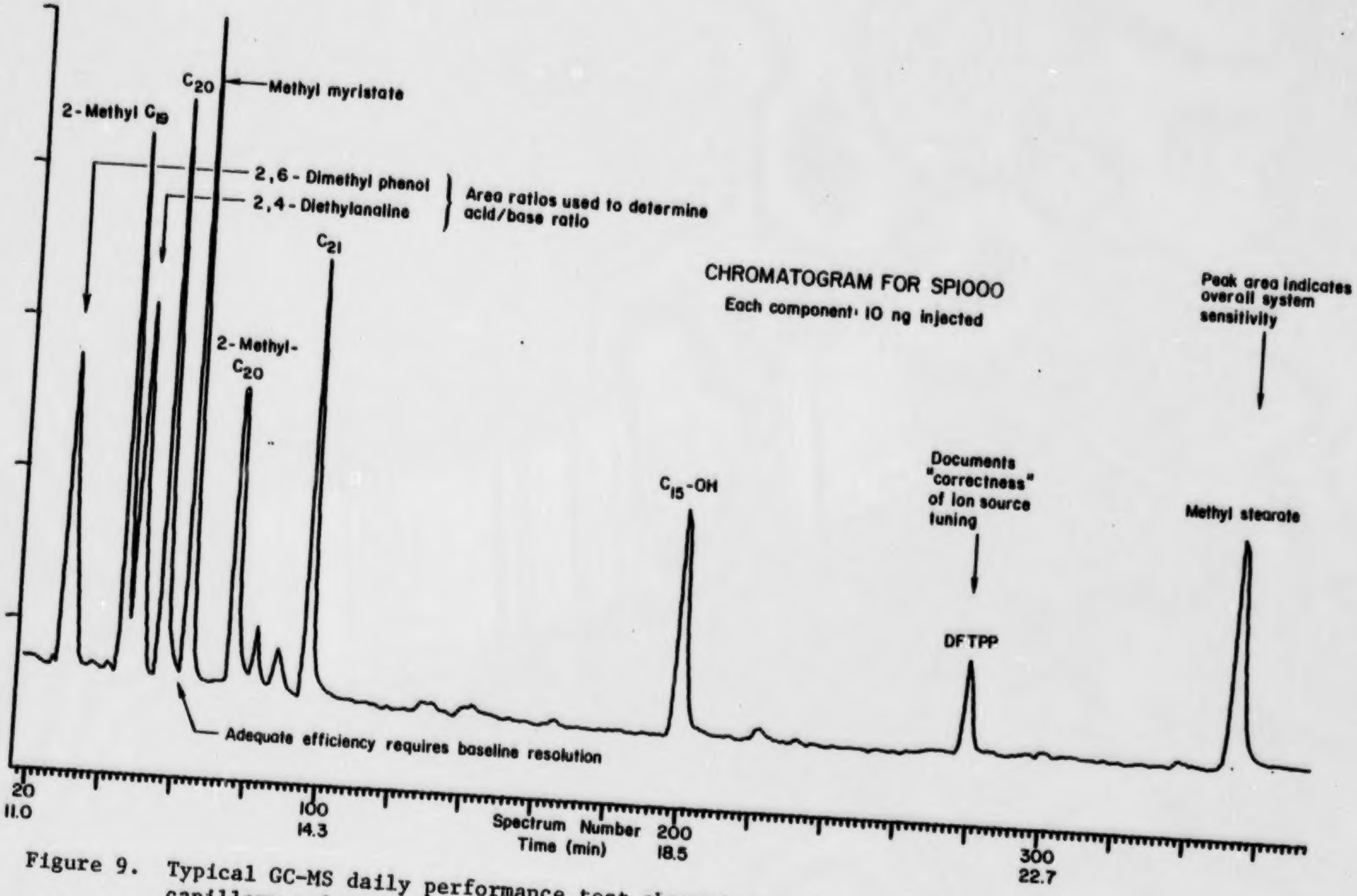

Figure 9. Typical GC-MS daily performance test chromatogram for the SP1000 (polar) capillary column.

Data Acquisition: Mass range: 40 - 450 amu

IFSS data acquisition parameters:

Maximum repeat count: 5
Samples/amu: 1
Repeat count before checking lower threshold: 2
Integration time: 2×10^{-3} sec
Lower threshold: 3
Upper threshold: 1
(The above conditions give a slightly variable scan time--depending on collected ion current--of 2.4 ± 0.3 sec/scan)

Signal Amplification: Preamplifier: 10^{-8} Amp/Volt

Electron multiplier voltage: sufficient for 10^4 gain.

Controlled Temperatures: Separator oven and transfer line: 250° to 265°C for the SP1000 column and 265° to 285°C for the SP2100 column.

Analyzer manifold: 85° to 100°C

GC-MS DATA PROCESSING

Archival

All GC-MS data associated with concentrate analysis were archived on 9-track magnetic tape. The archived GC-MS data files include those for all system performance verifications (FC-43 calibration check, DFTPP check, and SGCSM check), analyses (including all replicate analyses) of concentrates, fractions, process blanks, and confirmation and quantification standards. A total of 89 2400-foot 9-track magnetic tapes were used for this purpose. The MS data system used for data acquisition was limited to a maximum of six digits for each file name. A file naming system was designed which prevented any redundant usage of file names and also coded the identifying characteristics of each sample. The coded characteristics were:

- The sampled city
- The sampling sequence of the city
- The type of concentrate (i.e., how it was produced)
- The GC column used
- The identity of the sample (i.e., unpartitioned concentrate and the various fractions)
- Whether the sample was a process blank
- Identification of each of the three GC-MS performance verification checks and the data file to which it corresponded

- Identification of an analysis of a standard mixture

Since use of the data file naming system is required in accessing the data on the 9-track tapes, it was fully described in each of the concentrate analysis reports and in Appendix C of this volume. Only the first three characteristics above (city, sequence, and type of concentrate), are used in discussions of the results in this Final Report. The tape-handling software which was written for this purpose has been supplied to the Project Officer (see Appendix A).

Correction for the Process Blank

Concentrate samples were partitioned individually rather than in batches, and a set of process blank samples were generated simultaneously in parallel fashion. The process blank samples were analyzed by GC-MS in sequence with the corresponding sample fractions and the blank data were processed exactly as the sample data. Components of the sample fractions that were present as fractionation artifacts were identified by correlating the blank data with the sample data. In this correlation, the analyst attempted to find every discernible component of the corresponding process blank in the sample data by comparing chromatographic retentions and mass spectral characteristics. Sample constituents which were thereby identified as artifacts due to the partitioning process were not reported as being present in the sample. The only exceptions to this rule occurred for compounds which were present at higher concentrations (by at least a factor of 5 to 10) in the sample and which were not unexpected sample components (for example, plasticizers). Borderline cases were indicated "partially in the blank" in the tables of the individual concentrate reports which identified the GC peaks, but these compounds were not entered in the computer-managed data base of identified compounds.

Compound Identification and Confirmation

Tentative Identification of Sample Components--

Generally, compounds were tentatively identified based on a computerized or manual comparison of the compound mass spectrum with a library of reference mass spectra. In some cases, identification by manual interpretation was performed if it could be done cost-effectively. Appropriate background spectra were subtracted from the sample constituent mass spectra used for identification. Background corrected mass spectra normally corresponded to the top of each discernible GC peak.

Three different mass spectral matching computer programs were available for use in this work: two used a Systems Industries System/150 data system and Battelle-developed software and one used a Finnigan/INCOS 2400 data system. Since the Finnigan/INCOS mass spectral matching program correctly identified mass spectra more reliably than the other two programs and provided the most convenient data output format, the System/150 processing New software was written to enable the transfer of background corrected mass spectra from the System/150 data system to the INCOS data system (Appendix A). The data base for the computer matching system included the most recently released mass spectral library from the National Bureau of Standards (31,357 spectra). In addition, software was written to bring each new version of the library into use in advance of commercial availability through the Finnigan Corporation (Appendix A).

Confirmation of Tentative Identifications--

A compound identification was considered tentative unless it could be confirmed by comparison of mass spectrum and relative retention time with the corresponding data obtained on an authentic reference sample analyzed under the same GC-MS conditions. The status of a compound identification is indicated in the tabular computer output with either a "T" (for tentatively identified) or a "P" (for positively identified, i.e., confirmed).

Tentative identifications had to meet the following criteria to qualify for confirmatory activity:

1. The compound was not a known artifact of sample processing.

2. Identification confidence level of the senior analyst was about 80 percent or greater.

3. The compound was commercially available for about \$15 or less. In the case of compounds with higher interest functional groups, the upper price limit was in the \$20 to \$30 range. For compounds of probable health effect significance, there was no upper price limit. (The decision to purchase compounds at greater than \$20 per sample was made by the project principal investigator with input from the Project Officer in special cases.)

Sources were sought for tentatively identified compounds which met the first two criteria above. Battelle's in-house sources were searched before resorting to commercial suppliers. The main approach for commercial procurement was to request quotations for the minimum quantity from the most likely possibilities listed in the current volume of Chem Sources-USA (Directories Publishing Co., Inc., Ormond Beach, Florida). The Chem Sources-USA editions published in 1978, 1979, and 1980 were used for this work. Reference compounds were purchased according to the third criterion above.

Neat reference standards were used as received without first checking purity or verity. In general, purity was not a primary concern since the data generated were not to be used for quantitative purposes. When the GC-MS data indicated problems with purity or verity the compound was either rejected from the confirmation database, or further work was done to establish the verity of the data for compound identification confirmation purposes. Solutions of neat reagents were prepared individually at 5 mg/ml in methylene chloride or hexane, depending on compound polarity. Free acids and other high polarity compounds were dissolved in methanol. Other solvents were used only as required by solubility problems. Aliquots of 30 to 50 individual standards were mixed using microsyringes and diluted with hexane or methylene chloride to a concentration of 10 to 20 μg/ml. Mixtures of free acids including phenolic compounds were methylated before GC-MS analysis using diazomethane exactly as for concentrate acid fractions. Internal standard (2.0 μg hexaethylbenzene) was added, and the mixture was analyzed by GC-MS exactly as for the concentrate sample fractions and blanks.

Background subtracted spectra of all discernible GC peaks and shoulders were plotted and library matched (using Finnigan INCOS software). The data were correlated with the known composition of the mixture. Discrepancies with INCOS match results, ambiguities concerning isomer assignment or other indications of questionable purity or verity of individual compounds were reconciled by using the compound in question in a subsequent mixture of different composition. Often, chemically related species were used in the same mixture at concentrations different by integer factors to aid in assignment of component identities. The resulting standard mass spectra were catalogued for future reference and the GC and other relevant parameters were entered into the computerized database. In all, GC data for 1050 individual compounds were entered in the mainframe computer database. Software was written which supplied listings of these compounds and the corresponding retention data ordered by four different criteria:

- Increasing Molecular Weight
- Increasing Relative Retention on the SP1000 GC Column
- Increasing Relative Retention on the SP2100 GC Column
- Increasing Inventory Index Number of the EPA Reference Standard Repository

A set of these four listings in their final form constituted one of the deliverables required by the contract (see Appendix A).

In confirmation of tentative identifications, the acceptance criteria for GC retention was correspondence of relative retentions within 0.1 percent to 1 percent, depending on the proximity of elution to that of the internal standard, hexaethylbenzene. Generally, GC relative retentions over the range 0.3 to 1.8 agreed with reference data within about 0.5 percent. In some cases, GC retention data for concentrate samples showed a systematic drift in the GC retentions for the deuterated internal standards and/or other components identified at high confidence levels. This drift was taken into account when comparing sample GC retention with the confirmation database.

Aliquot for EPA's GC-MS Reference Standard Repository--

A portion of each neat standard was reserved to establish an EPA GC-MS reference standard repository. Screw-cap vials (2.75 ml) with Teflon-lined septa seals were filled at least half full or with half of the total material purchased (whichever was greater) and labeled with the compound name, formula, commercial source, and an inventory index number. Compounds indicated to be temperature sensitive were stored at -10° until transferred to U.S. EPA HERL-CI. Compounds of known health hazard were stored separately from the others.

Computerized GC-MS Data Searching for Specified Compounds

In addition to identifying the mass spectra obtained for discrete GC peaks and shoulders, a more sensitive computer search system was used to detect the presence of 53 specific compounds (listed in Table 4) considered by the

TABLE 4. LIST OF THE 53 COMPOUNDS FOR WHICH GC-MS DATA WERE SEARCHED

Compounds Listed by Increasing Molecular Weight
Chloroprene
Aniline
Phenol[a]
Diethylnitrosamine
Styrene
4-Methylphenol
2-Methyl styrene
2,4-Diamino toluene
2,4-Dimethylphenol
Nitrobenzene
2-Chlorotoluene
2-Chloroaniline
3-Nitroaniline
4-Chlorophenol[b]
2-Naphthylamine
1,4-Dichlorobenzene
p-Nitrophenol[b]
4-Chlorophenyl methyl ketone
2-Chloronaphthalene
Diphenylamine
4-Phenylaniline
2,4-Dichlorophenol[b]
1,2,4-Trichlorobenzene
2,4-Dichloronaphthalene
Fluoranthene
2,4,6-Trichlorophenol[b]
2-Methyl-4-chlorophenoxyacetic acid[b]
N-Phenyl-1-naphthylamine
Chrysene
2,4-Dichlorophenoxyacetic acid[b]
1,4-Dibromobenzene
Benzo(a)pyrene
Benzo(b,k)fluoranthene
Hexachloro-1,3-butadiene
Pentachloroaniline
2,4,5-Trichlorophenoxyacetic acid[b]
Hexachlorocyclopentadiene
Benzo(ghi)perylene
Indeno(1,2,3-cd)pyrene
Pentachlorophenol[b]
Hexachlorobenzene
Lindane
Tetrachlorobiphenyls
Pentachloronitrobenzene
Pentachlorobiphenyls
Triphenyl phosphate
DDT
Hexachlorobiphenyls
Aldrin
Tri-(m)-cresyl phosphate
Heptachlor
Dieldrin
Hexabromobiphenyl

a) Searching for both the free acid and the methyl ether was performed.

b) Searching for the methyl ether or methyl ester only was performed.

Project Officer as possibly significant health risks. For this purpose, a highly sensitive and specific computer search program was developed for use with the System/150 GC-MS data system. In this program the technique of selected ion summation (SIS) was used to search for each of the 53 compounds within specified relative retention time windows (8). The program was very effective at detecting and locating the specified compounds in the GC-MS data even when the compound mass spectra were hidden by ion current signals from background and co-eluting compounds. The main features of the SIS program are given in Appendix A.

An important quality assurance measure was that mass spectra of SIS search "hits" were always manually verified before the data were reported to insure against false positives due to co-elution interference. The SIS search compounds (Table 4) which were detected appear in all computer-printed tables with an asterisk flag (*) in front of the compound name and a concentration entry in ng/l which replaces the "P" or "T" indicator in the tables showing compound identification status as confirmed or tentative.

Quantification of Identified Compounds

In principal, each of the 521 individual compounds for which compound identifications in DW and AWT concentrates have been confirmed (and, therefore, for which a reference standard of the compound was on hand) could have been quantified using ordinary response factor/internal standard methodology. However, such an approach would not be cost-effective since many of these compounds with confirmed identification have little or no known health effect significance. Nevertheless, it was important to have some basis for approximating the concentrations of each of the 1641 individual tentatively and positively identified compounds. Two approaches to quantitative approximation were used as the best compromise for this problem:

(1) The 53 compounds of Table 4 which were detected by the SIS specific search software were quantified using deuterated internal standards, extracted ion current profiles (EICPs) and response factors generated from GC-MS analysis of standards.

(2) The concentrations of all other tentatively or positively identified compounds were approximated by comparing the size of the GC peak in the total ion chromatogram with that of the pre-analysis internal standard, hexaethylbenzene, to generate a relative size (RS) parameter.

Quantification of Specific Search Compounds--

Response factors (RFs) were generated, as required, for the 53 compounds of Table 4 using the data from GC-MS analyses of standard mixtures of these compounds which were processed through the concentrate partitioning scheme. Equation 1 shows the formula used to generate the response factors for the component "A" relative to an internal standard (IS):

$$RF_A = \frac{\dfrac{\text{Amount A } (\mu g \text{ in std})}{\text{EICP area (A in std)}}}{\dfrac{\text{Amount IS } (\mu g \text{ in std})}{\text{EICP area (IS in std)}}} \qquad \text{Eq. 1}$$

Quantification of component "A" in the GC-MS sample data was then performed using equation 2:

$$\text{Amt. A } (\mu g \text{ in sample}) = \frac{\text{EICP area (A, sample)}}{\text{EICP area (IS, sample)}} \times RF \times [\text{Amt. IS } (\mu g \text{ in sample})] \qquad \text{Eq. 2}$$

Equation 2 is equivalent to the use of a one-point plus the origin standard curve, and it requires that the same EICP masses used to determine the response factor (RF, eq. 1) also be used to generate the EICP peak areas in the GC-MS data for the concentrate. Note also that best results are be obtained when the instrument high mass/low mass response characteristics are identical for both the concentrate and standard mixture data acquisitions. As mentioned above, this tuning characteristic was checked using DFTPP prior to every GC-MS acquisition. In addition, care was also taken to ensure that none of the ion current signals used in the area calculations were saturated.

In theory, optimal quantification would result from analysis of the unpartitioned concentrate since ambiguities due to the nonreproducibility of losses of the designated analyte and/or deuterated internal standard in the partitioning scheme are automatically avoided. In practice, however, the high dilution factor and extremely complex composition of the concentrate, as received, always resulted in more sensitive detection and higher quality data for SIS specific search and quantification on the fractions. Nevertheless, the GC-MS data from all the analyzed unpartitioned concentrates (which excludes the concentrates produced by XAD-2 extraction of RO brine) were searched for the compounds of Table 4 using the SIS software, and quantification was performed using that data whenever possible. Response factors generated from an unpartitioned standard were used in these cases. Often, the quantitative data from the unpartitioned analysis were too weak to serve any purpose other than a confirmatory one for the results from the fractions, and in these cases quantification was performed using the fraction data.

Semi-quantitative Estimation by Relative Size (RS) of the GC Peak--

The relative size (RS) parameter was developed as a somewhat imprecise but extremely cost-effective method for estimating the amount of every identified component. It is a logarithmic scale spanning four orders of magnitude. Assignment involved visually estimating the size of each GC peak in the total ion current chromatogram relative to that of hexaethylbenzene, an internal standard of which 2 µg were added to every sample immediately before GC-MS analysis. Thus, each GC peak corresponding to an identified compound was assigned an RS value consisting of an integer from 1 to 9 on the basis shown in Table 5.

The computer report-generation software normalized all RS values (before outputting) to a typical 1514-liter sample according to equation 3:

$$\text{RS (output)} = 2 \log_{10} \left[\frac{\text{antilog}_{10}[\text{RS(input)}/2]}{(\text{liters sampled})/(1514 \text{ liters})} \right] \qquad \text{Eq. 3}$$

Thus, computer output RS values in Tables 9, 10, and 11 are directly comparable from one concentrate to another in terms of being representative of concentrations in the original water. Generally, the output RS values ranged between 0 and 9. However, when the sampled water volume exceeded 1514 liters, it was possible for the RS (output) value, Eq. 3, to become negative for the smallest RS (input) values since the scale is logarithmic. The RS value was designed to provide approximate quantification for every water concentrate sample component identified. While it might be tempting to assign the corresponding value in nanograms per liter of original water to each compound (as indicated in Table), such an assignment would not be scientifically well founded, and it also could be misleading and easily misinterpreted. If the following conditions prevailed, then the RS criteria would have provided exact quantification:

- The sample component and internal standard had the same response factor for mass spectrometric detection

- Instrument response was linear through the entire 10,000 fold RS range

TABLE 5. GC PEAK RELATIVE SIZE (RS) VALUES FOR SEMI-QUANTITATIVE ESTIMATION OF COMPOUND CONCENTRATIONS

RS Value	GC Peak Size Relative to the Internal Standard[a]	Approximate Concentration[b]	
9	Greater than 100X	>1300 ng/l	1.3 ppb
8	30 to 100	.	.
7	10 to 30	.	.
6	3 to 10	.	.
5	1 to 3	13 ng/l	13 ppt
4	1/3 to 1	.	.
3	1/10 to 1/3	.	.
2	1/30 to 1/10	.	.
1	1/100 to 1/30	0.13 ng/l	0.13 ppt

a) The ranges are half orders of magniture so the RS value numbers span a "linear" log range. Technically, they should be 1-3.16, ...31.6-100, etc., but for visual comparison purposes only one significant figure is more appropriate.

b) Assuming the GC-MS response factor for the analyte to be equal to that of the Internal Standard and a 1514 liter (400 gallon) water sample. See text for other precautions concerning the use of the RS value.

c) ppb: parts per billion; ppt: parts per trillion.

- Neither the identified component nor internal standard GC peaks were broadened due to chromatographic overloading

- The sample component was recovered quantitatively through the partitioning scheme and suffered the same relative chromatographic losses as the internal standard

- The component was removed from the original water into the concentrate quantitatively.

Clearly the preceding conditions were never met. However, since detection of the internal standard was probably acceptably reproducible, direct comparison of RS values for the same component from one concentrate to another can be made with relative confidence. While it is known that RO recovers many organic species nearly quantitatively (especially those of high molecular weight) it may be somewhat less efficient for others. In addition, the residue weight results of Tables 7 and 8 (see Section 5, Results and Discussion) indicate that significant amounts of organic material were not recovered in the partitioning scheme. These and other factors giving rise to the underestimation of concentration based on the RS value (as per Table 5) are expected to generally outweigh other factors which cause overestimation. Thus, the correlation of concentration with RS value as indicated in Table 5 should be taken as a lower bound only.

DATA MANAGEMENT

The enormous bulk of compound identification results and other data generated by analyses of the DW and AWT concentrates could not be managed efficiently by manual means. An existing system of Battelle-written software described as a numerical classification and evaluation system (NUCLEUS) for large bodies of related information, was modified for this purpose. The NUCLEUS software was operated on three CDC computers (Control Data Corporation; Cyber 6500, Cyber 73, and Cyber 74) in Battelle's central computing facility. This software featured:

- A structured programming language
- Dynamic simulation modeling
- Data base management
- Report generation
- Conversational programs
- Batch or on-line access (via remote terminal in the laboratory) for program modification and data entry or editing.

The NUCLEUS data management system provided a number of extremely valuable capabilities:

- Flexibility in the way all lists of identified compounds could be ordered

- Combining, non-redundantly, related lists of identified compounds for a concentrate

- Combining, non-redundantly, lists of compounds for up to 27 concentrates

- Tabulating occurrence and concentration (RS value) statistics of 25 types of molecular functional groups for individual fractions, combinations of fractions and combinations of concentrates

- Incorporating useful, descriptive information about the individual compounds.

These capabilities were necessary for the achievement of the project goal of enabling interpretation of the biological activity testing results in terms of the chemical composition of the concentrate. A further benefit was the ability to produce error-free listings of compound identification results which were organized in multiple, useful formats. With over 2100 different identified compounds entered in the data base, it is clear that a computer-assisted data management and report generation system was the only reasonable approach to this problem.

The data base stored the following information relevant to each compound identification:

- Fraction and concentrate in which identification occurred
- GC phase used
- Retention time
- Relative retention value
- Spectrum number
- Relative size of the GC peak
- Concentration (ng/l in original water), if available
- Status of the identification (tentative or confirmed)
- Description of the compound including:

    1. Systematic name
    2. Common name
    3. CAS number
    4. Molecular weight
    5. Molecular formula
    6. Industrial source and/or use
    7. Classification as one of ten chemical types
    8. Functional groups contained in the molecule.

Once these eight items describing the compound have been entered, identification in subsequent concentrates require entry of only the CAS number and the other non-compound descriptive items listed above.

In addition to the above listed information relative to each identified compound, the following general information was also entered into the database:

- Descriptive data for the concentrate (city, date of sampling and volume of water, date received, date of partitioning and name of the person who partitioned the concentrate, the volume, color and solvent of the concentrate, as received, and the amount of the concentrate reserved for unpartitioned analysis)
- Residue weight analysis data for the fractions and unpartitioned concentrate
- Conditions used for the GC-MS analysis.

The above items provided the necessary information for computer data processing and generation of the computer-printed tables contained in the individual concentrate analysis reports and those presented in this Final Report.

REPORT GENERATION

Concentrate Analysis Reports

Separate reports on the GC-MS analysis results for each DW and AWT concentrate were prepared and delivered to the Project Officer. These reports, along with other relevant information, are tabulated in Tables 1A and 2A of Appendix A. Each complete concentrate analysis report consisted of seven volumes produced in various numbers of copies. The contents of each volume are described in Table 6. Volume 1 was designed to contain the core material of the concentrate analysis report. The computer-printed tables selected for inclusion in that volume were the following:

- All compounds found in all four of the GC-MS analyzed fractions in non-redundant listings of three tables:

    1. by decreasing size of the GC peak (RS value) showing the fraction(s) and GC column(s) where the identification was made, the status of the identification (tentative or confirmed), the RS value and when known the concentration in ng/l.

    2. ordered as in 1 above, but showing both systematic and common names, industrial source or use, molecular weight and RS value.

    3. ordered by increasing molecular weight showing molecular formula.

TABLE 6. CONTENTS OF THE INDIVIDUAL REPORTS FOR DW AND AWT CONCENTRATES

Volume	Contents	Number of Delivered Copies
1	Short summary of the results Analytical scheme Residue weight results for fractions and the unpartitioned concentrate Discussion of the results Labeled GC-MS chromatograms for the unpartitioned concentrate (both GC columns) Key computer-printed listings of compound identification results[a]	15
2	Complete set of computer-printed listings of compound identification results[a] Labeled GC-MS chromatograms of the four fractions (both GC columns)	3
3	Mass spectra of compounds with confirmed identification and tentative identification found on the SP1000 GC column	3
4	Mass spectra of compounds with confirmed identification and tentative identification found on the SP2100 GC column	3
5	Mass spectra of the deuterated internal standards from the analyzed fraction data GC-MS chromatograms of a standard run of the compounds for specific search on SP1000 and mass spectra of specific search "hits" on SP1000 GC-MS chromatograms of a standard run of compounds for specific search on SP2100 and mass spectra of the specific search "hits" on SP2100	3
6	Mass spectra of decafluorotriphenylphosphine (DFTPP) ion source tuneup verification Standard GC separation mixture (SGCSM) GC-MS system performance verification chromatograms Labeled GC-MS chromatograms for analyses of fractions of the partitioning process blank	1
7	Real time total ion chromatograms of concentrate fractions on SP1000 and SP2100 GC columns	1

a) See text for an itemized listing of these tables.

- Functional group listings for all four analyzed fractions combined as follows:

    1. all results from the SP1000 GC column showing total, maximum and minimum RS values

    2. all results from the SP2100 GC column showing total, maximum and minimum RS values

    3. results from both columns combined without RS value information

- Identified compound listings for the four fractions, individually, but showing combined results from analysis on both GC columns; ordered by decreasing RS value

- Functional group listings for the four fractions, individually, but showing combined results from both GC columns.

These tables were also included in the second volume along with the following tables which comprised the entire set of computer-produced tabulations:

- Identified compounds for each of the four fractions on each of the two GC phases (eight sets of tables) with each list ordered three different ways:

    1. alphabetically; showing molecular formula, molecular weight, identification status (tentative or confirmed) and concentration in ng/1, if known

    2. by increasing relative GC retention; showing GC retention time, relative GC retention, spectrum number, RS value, and identification status

    3. by decreasing RS value; showing RS value, identification status and concentration in ng/1, if known known

- Functional group listings for each of the four fractions on each of the two GC phases (eight tables).

Combined Concentrate Analysis Reports

Whenever a concentrate report was the final one of a series of related concentrates, all the results of the related series were integrated by the NUCLEUS data processing software into a single, tabular output for presentation as a composite report. These non-redundant listings were produced in two correlated tables. The first table displayed all results in a listing of common names ordered by decreasing relative GC peak size. For each entry, this table showed:

- the concentrate in which the detection occurred
- the status of the identification (confirmed or tentative) in each concentrate
- the concentration (ng/l) results, if known
- the largest relative GC peak size found for the compound in each concentrate
- an indicator symbol marking compounds of special interest.

Whenever the number of combined concentrates exceeded six, this first table was presented in two parts. The second correlating table showed, for each entry of the first table, the corresponding systematic name, CAS number, molecular formula and molecular weight. The concentrate reports which contained these special, combined reports as well as the concentrates which have been combined, are designated in Tables 1A, 2A, and 3A of Appendix A. In all, 15 such combined reports were produced for inclusion in the regular concentrate reports.

Special Listings of the Databases

The NUCLEUS software for data management also provided facile production of highly useful listings of the entire identified compound database. These listings did not indicate the concentrate in which detection occurred, but instead, they showed chromatographic and other information. These lists were useful in determining whether compounds identified in concentrates were already in the database. They were also useful for comparing GC retention values to those previously observed. The identified compound listings were produced in two formats: (1) all compounds ordered by increasing molecular weight, and (2) all compounds ordered by increasing relative GC retention. The latter was produced in two sets of tables--one set for each GC phase (SP1000 and SP2100). Each of these sets were, in turn, composed of two tables: (1) compounds that were identified in the derivatized acid fractions, and (2) compounds that were identified in the other three GC-MS analyzed fractions (i.e., base-neutrals).

The database of compounds identified in concentrate samples was distinct from the database of compounds analyzed as reference standards for confirmation of identifications. This confirmation database was also listed for utility purposes in four tables which are described earlier.

Since these utility listings of the two databases were valuable beyond the scope of this work as general reference collections, they were provided to the Project Officer in updated versions through the course of the project work. These listings are tabulated and described in more detail in Appendix A. The identified compound database listing ordered by molecular weight is included as Appendix D. This list has been correlated with the key tables which show the occurrence of the compounds in the samples.

SUGGESTIONS FOR IMPROVEMENTS TO THE ANALYTICAL SCHEME

Some minor modifications to the Analytical Scheme presented above can be recommended based on the two years of experience with this program.

Internal Standards

At the beginning of the research program all commercially available and applicable deuterated internal standards were obtained. In addition, one internal standard, dimethyl terephthalate-D_4, was synthesized since there was no commercially available deuterated standard of correct polarity for recovery in the high polarity fraction. Future applications of the analytical scheme should incorporate some of the additional deuterated compounds which have recently become available. In particular, additional compounds with a variety of functional groups should be selected to provide more internal standards in the medium and high polarity fractions. Nitriles, alcohols, esters, amides, amines, ketones aldehydes and non-aromatic acids are recommended to fill these internal standard gaps.

Concentrate Fractionation

The low number of basic substances found in the concentrates suggests that the separate step of extraction of these species should be omitted. Moreover, modern glass capillary GC columns allow gas chromatography of these materials without derivatization in nearly all cases. Good recovery of the bases from the silica gel column could be assured by a small amount of methyl amine modifier in the methanol used to elute the high polarity fraction.

Derivatization of the acids using gas phase delivery of diazomethane was excellent with respect to minimizing the introduction of impuritites via the derivatization reagent. However, in situ formation of chloroalkanes (apparantly due to multiple CH_2 insertions on an active precurser) was a poorly understood and controlled problem. Solvent exchange removal of methylene chloride solvent and addition of a trace quantity of mineral acid prior to derivatization appeared to be a reliable solution, but more work should be performed to refine this critical step.

Final sample evaporation on the N-Evap® apparatus was tedious, time consuming and difficult to maintain at optimum conditions. This procedure should be replaced with another which is better optimized regarding reliability and speed.

GC-MS Data Acquisition

Newer GC-MS equipment is capable of faster, more reliable scanning of the mass range. This capability can be exploited through the use of H_2 GC carrier gas and marginally faster temperature programming (perhaps 3°C/min) without any detriment to the chromatography or quality of the mass spectral data. Experience suggests that a shorter scan range (40 amu to 350 amu) would also enable higher quality mass spectral data with almost no loss of compound identification capability. Repeating an occasional analysis whenever the data suggested higher mass ions were present would probably still allow a cost-effectiveness improvement.

Data Processing

Improvements in mass spectrometry data systems now allow the flexible creation of specialized GC-MS data processing routines. Two recommended improvements to the analytical scheme which this new capability would enable are the following:

- Capability to build a mass spectral library of the unidentified mass spectra of each analysis would enable the accurate and facile updating of compound identification results once recurring unidentified mass spectra are successfully interpreted. In addition, the cataloguing of occurrences of such unidentified mass spectra would provide the necessary occurrence frequency and concentration level information on which to base decisions concerning the investment of resources in pursuing manual interpretation

- A valuable automated QC step should be incorporated in which, at the end of each GC-MS data acquisition, a search routine would generate raw areas of all the pre-fractionation deuterated internal standards and any pre-analysis internal standards and calculate the appropriate ratios between the former and the latter. This hard-copy QC report would allow essentially "real-time" QC monitoring of both the GC-MS system performance and the recovery effectiveness of the fractionation scheme.

SECTION 6

RESULTS AND DISCUSSION

ORGANIZATION OF THE PRESENTATION

Presentation and discussion of the analysis results for the DW and AWT concentrates is organized in four sections:

1. A general overview of the analysis results, approach to the concentrate production process blank problem and summary of the available tabulations (Tables 7 and 8)
2. Discussion of the DW results (Table 9)
3. Discussion of the AWT results (Table 10)
4. Comparison of DW and AWT results (Table 11).

Items 2, 3, and 4 each have an associated computer-printed listing of the identified compounds showing the concentrates where detection occurred, the relative size of the GC peak for each detection and an indication of the compounds which should be considered as attributable to the RO processing blank or the XAD-2 resin adsorption/elution blank. These tables are very long (30, 35, and 37 pages for DW (Table 9), AWT (Table 10), and combined DW and AWT (Table 11), respectively) and have been placed together at the end of this section to facilitate referral by the reader.

OVERVIEW OF THE RESULTS

Comparison of Residue Weight Results and Compound Identification Statistics

Distribution of Organic material in the Analyzed Factions--

Residue weight analysis results and compound identification statistics are shown for DW concentrates in Table 7 and for AWT concentrates in Table 8. Comparison of the residue weight results in Tables 7 and 8 shows a similar predominance in both types of water sources of acidic and highly polar neutral materials in the recovered fractions. Composited values for the four Lake Tahoe, three Pomona (9/25/74) and two Blue Plains (9/20/74) concentrates, Table 8, have been taken for these three samplings as approximations of the total organic material recoverable from the RO brines by solvent extraction. Concentrates C3C, R1C, R2C, E1C, and B2C consisted of composites of all RO brine solvent extracts (see Section 2 and Table 2). Thus, concentrates C2N and D2N, Table 8, are the only sets of data not useable for comparison as a combined solvent extract of the RO brine produced by a given sampling.

TABLE 7. PERTINENT CONCENTRATE DATA FOR DRINKING WATER

			Residue Weight Analysis						Identification Results Number of Compounds						
				Fractions, %[c]					Status				Special Compounds		
City	Code[a] Name	Date and Volume Sampled (Liters)	Concentration[b] µg/ℓ	Acid	Aromatic	Medium Polarity	High Polarity	Total %[d] Recovered	Confirmed	Tentative	Total[e]	Unidentified[f]	Specific[g] Search	Consent[h] Decree	Industrial[i] Indicators
Poplarville, Mississippi	V1C	3/2/79[j] (15,100)	0.6	2.4	0.6	4.1	11	22	19	31	50	33 41	4	9	9
Poplarville, Mississippi	V1X		17	1.8	21	1.0	1.8	38	60	98	158	110 123	3	6	6
XAD-2 Diethyl Ether Elution Blank	T2B	(k)	—	0.07[l]	0.07[l]	0.02[l]	0.04[l]	—	42	57	99	74 52	2	7	11
Cincinnati, Ohio	T1C	10/17/78[j] (1,460)	143	32	0.05	1.6	18	52	66	85	151 (140)	152 53	6	7	9
Cincinnati, Ohio	T1X		397 540	11 17	0.0 0.0	0.2 0.6	1 5.5	12 23[m]	35	42	77 (66)	69 32	1	5	2
Cincinnati, Ohio	T1Y		527	23	0.2	1.3	16	41	126	117	243 (211)	121 99	19	13	24
Cincinnati, Ohio	T4C	1/14/80[j] (5,300)	115	26	0.1	0.3	10	36	112	81	193 (165)	73 64	16	13	17
Cincinnati, Ohio	T4X		745	10	0.03	0.1	0.6	11 14[m]	96	85	181 (113)	64 73	7	7	5
Miami, Florida	M2C	2/3/76[j] (2,280)	527	38	0.1	0.3	11	50	77	143	220 (208)	84 42	6	12	13
Miami, Florida	M2X		2,100	11	0.4	0.2	0.6	13 20[m]	66	173	239 (106)	99 47	2	8	6
New Orleans, Louisiana	N2C	1/14/76[j] (6,620)	217	31	0.5	6.0	16	53	101	148	249 (231)	55 59	12	15	15
New Orleans, Louisiana	N2X		949	9	0.3	0.2	0.7	10 18[m]	75	158	233 (144)	180 114	3	10	8
Philadelphia, Pennsylvania	P2C	2/10/76[j] (5,810)	177	31	0.3	0.6	32	65	125	167	292 (279)	51 46	10	11	18
Philadelphia, Pennsylvania	P2X		1,006	5	0.1	0.4	2	7.7 19[m]	96	125	221 (114)	61 33	4	11	8
Ottumwa, Iowa	O2C	9/10/76[j] (5,450)	139	39	0.1	0.5	17	57	83	150	233 (213)	52 57	6	8	12
Ottumwa, Iowa	O2X		775	6	0.1	0.1	0.5	6.7 14[m]	70	161	231 (142)	49 37	3	6	7
Seattle, Washington	S2C	11/5/76[j] (11,750)	37	30	0.4	1.5	20	53	120	269	389 (361)	68 50	11	12	15
Seattle, Washington	S2X		99	8	0.1	0.1	3.3	12 23[m]	70	101	171 (140)	60 28	7	8	12
Extraction Solvent Blank	X1C	(k)	—	0.05[l]	0.00[l]	0.02[l]	0.03[l]	—	19	33	52	28 29	0	2	5
XAD-2 Ethanol Elution Blank	X1X	(k)	—	0.04[l]	0.09[l]	0.08[l]	0.09[l]	—	27	31	58	80 62	0	4	2

a) The three digit code name is used in the computer generated listings.
b) The amount of organic material in the concentrate expressed as µg/l (ppb) in the original water sample.
c) The amount of the recovered fractions, expressed as a percentage of the concentrate (residue basis). The aromatic, medium polarity, and high polarity fractions are the hexane:benzene, methylene chloride, and methanol silica gel eluates respectively.
d) Includes the recovered alkane/alkene fraction (hexane silica gel eluate) which is not analyzed by GC-MS.
e) The value in parentheses excludes compounds attributable to the RO process blank or XAD-2 resin (see discussion in Volume 1).
f) Unidentified components are listed separately for each GC phase. Upper number: SP1000. Lower number: SP2100.
g) The 53 compounds for which the data are specifically searched are listed in Table 4 (Volume 1).
h) The EPA "Consent Decree" list of priority pollutants (semi-volatile compounds).
i) The "Chemical Indicators of Industrial Pollution" list (Federal Interim Primary Drinking Water Regulations, February 9, 1978).
j) Concentrates which were derived from the same water sample or a duplicate water sample.
k) A blank which does not correspond to a water sampling.
l) The value shown is the fraction weight (mg) rather than the percentage of the concentrate.
m) The value shown is composited from the values for the solvent extract and XAD-2 extract concentrates.

TABLE 8. PERTINENT CONCENTRATE DATA FOR ADVANCED WASTE TREATMENT WATER

			Residue Weight Analysis						Identification Results Number of Compounds						
				Fractions, %[c]					Status				Special Compounds		
City	Code[a] Name	Date and Volume Sampled (Liters)	Concentration[b] μg/ℓ	Acid	Aromatic	Medium Polarity	High Polarity	Total %[d] Recovered	Confirmed	Tentative	Total[e]	Unidentified[f]	Specific[g] Search	Consent[h] Decree	Industrial[i] Indicators
Extraction Solvent Blank	X1C	(k)	—	0.05[ℓ]	0.00[ℓ]	0.02[ℓ]	0.03[ℓ]	—	19	33	52	28 29	0	2	5
Lake Tahoe, California	L2P	10/24/74[j] (1,500)	51	7.4	1.2	2.7	77	89	154	106	260 (240)	55 62	6	12	21
Lake Tahoe, California	L2M		52	65	0.02	4.9	20	90	71	62	133 (105)	54 48	5	4	12
Lake Tahoe, California	L2N		153	16	2.4	2.6	60	81	73	84	157 (136)	72 79	5	8	6
Lake Tahoe, California	L2D		50 306	39 27	0.01 1.4	0.8 2.7	21 50	61 81[m]	99	79	178 (166)	97 96	9	8	8
Pomona, California	C3C	6/17/75 (1,500)	87	7.7	1.2	3.0	34	46	63	51	114 (104)	56 55	9	5	14
Pomona, California	C1P	9/25/74[j] (1,500)	197	0.99	1.8	1.5	23	28	90	68	158 (143)	56 68	10	11	11
Pomona, California	C1M		104	22	0.96	1.9	13	38	83	70	153 (133)	96 61	10	11	11
Pomona, California	C1N		69 370	83 22	0 1.2	1.1 1.5	3.3 17	88 42[m]	82	113	195 (170)	117 70	11	9	13
Pomona, California	C2N	10/2/74 (1,500)	37	5.7	5.4	1.9	5.6	20	51	69	120 (106)	80 43	5	8	16
Orange County, California	R1C	1/27/76 (1,500)	104	6.6	0.7	0.5	28	37	78	47	125 (105)	99 65	1	6	7
Orange County, California	R2C	2/3/76 (1,500)	144	9.0	1.1	1.8	37	50	135	120	255 (233)	163 193	22	10	13
Escondido, California	E1C	7/8/75 (1,500)	18	2.3	0.7	0.2	20	23	32	24	55 (40)	64 46	5	5	11
Dallas, Texas	D2N	11/11/74 (1,500)	18	33	3.2	0.1	13	62	76	37	113 (92)	21 25	2	6	8
Blue Plains, Washington, D.C.	B2C	5/31/75 (1,500)	46	12	1.1	1.4	63	79	65	59	124 (97)	82 90	6	8	13
Blue Plains, Washington, D.C.	B1M	9/20/74[j] (1,500)	23	26	0.2	1.0	13	41	80	61	141 (117)	159 108	6	8	9
Blue Plains, Washington, D.C.	B1N		21 44	59 42	1.4 0.8	1.7 1.3	20 16	83 60[m]	65	61	126 (110)	148 72	5	5	3

a) The three digit code name is used in the computer generated listings.
b) The amount of organic material in the concentrate expressed as μg/l (ppb) in the original water sample.
c) The amount of the recovered fractions, expressed as a percentage of the concentrate (residue basis). The aromatic, medium polarity, and high polarity fractions are the hexane:benzene, methylene chloride, and methanol silica gel eluates respectively.
d) Includes the recovered alkane/alkene fraction (hexane silica gel eluate) which is not analyzed by GC-MS.
e) The value in parentheses excludes compounds attributable to the RO process blank (see discussion in Volume 1).
f) Unidentified components are listed separately for each GC phase. Upper number: SP1000. Lower number: SP2100.
g) The 53 compounds for which the data are specifically searched are listed in Table 4 (Volume 1).
h) The EPA "Consent Decree" list of priority pollutants (semi-volatile compounds).
i) The "Chemical Indicators of Industrial Pollution" list (Federal Interim Primary Drinking Water Regulations,, February 9, 1978).
j) Concentrates which were derived from the same water sample or a duplicate water sample.
k) A blank which does not correspond to a water sampling.
ℓ) The value shown is the fraction weight (mg) rather than the percentage of the concentrate.
m) The values shown are composites for the indicated sampling.

Averaging the total recovery percentages for each of these eight AWT composite concentrates or equivalent composite concentrate groups of Table 8 and similarly averaging these values for the seven DW solvent extract concentrates of Table 7, the same value (52 percent) is obtained for the AWT and DW concentrates. The majority of the recovered material for both DW and AWT concentrates was found in the two most highly water soluble fractions (acidic and high polarity) with the eight AWT composite concentrates (and groups, as above) averaging 94 percent of the recovered material in these two fractions and the seven DW composite concentrates yielding a corresponding value of 97 percent. However, the distribution of these highly water soluble organic materials between acidic and neutral species is reversed for AWT versus DW concentrates: of the organic material in the AWT concentrates, averages of 16 and 33 percent were recovered in the acid and high polarity fractions, respectively, while, for the DW concentrates, these averages were 32 and 18 percent for the same fractions.

Comparison of the Amounts of Organic Material Present in DW and AWT Concentrates--

As cited above, only 5 of the 16 AWT concentrates shown in Table 8 were composites prepared by combining all six of the solvent extracts of each RO processing (sampling event). The other 11 AWT concentrates were individual solvent extracts which represent only part of the total material recoverable by solvent extraction of RO brine. Comparison of these AWT solvent extract composite concentrates (C3C, R1C, R2C, E1C, and B2C, Table 8) with the 7 DW solvent extract composite concentrates (T1C, T4C, M2C, N2C, P2C, O2C, and S2C, Table 7) shows that, generally, the sampled drinking water contained a higher concentration of organic material recoverable by the RO/solvent extraction procedure than did the AWT water. The average values in Tables 7 and 8 under "Concentration, µg/l" are 81 for the five AWT concentrates and 183 for the seven DW concentrates. Adding composite values for the Lake Tahoe, Pomona (6/25/74) and Blue Plains (9/29/74) samplings to the five AWT concentrates (as above) results in a somewhat higher average value of 140 µg/l although this value is still significantly less than the average for the seven DW concentrates. It cannot, however, be concluded that, on the average, the sampled AWT water contained less organic content than the sampled DW since additional concentrates of the RO brines were not produced using XAD-2 adsorption/elution for the AWT samplings. Indeed, the TOC data shown in Tables 1 and 2 are uniformly higher for the AWT samplings (Table 2) than for the DW samplings (Table 1) by a factor of two to four. Thus, the distribution of molecular polarities or other properties which have an impact on recovery by RO and/or solvent extraction of the organic species present must have been significantly different for these two water types. The tentative conclusion is that the AWT water contained higher relative amounts of more highly water soluble organic material with lower extraction efficiency than did the DW.

This conclusion seems to be supported by the statistics for the number of identified compounds for each concentrate in Tables 7 and 8. The average number of identified compounds for the 5 AWT composite solvent extract concentrates was 116 while the corresponding average for the 7 DW composite solvent extract concentrates was 228. This trend may also be explained simply by considering that, in all but one case (T1C, T1X, and T1Y; see Tables 7 and 8), the DW samplings involved greater volumes of water than those for AWT by factors ranging from 1.5 to 7.8. A larger volume of sampled water might be expected to yield detection limits at lower concentrations, and, indeed, the largest number of compounds (361) were detected for the concentrate with the greatest DW volume sampled (11,750 liters for Seattle, Washington, code S2C).

XAD-2 Resin Extraction Effectiveness/Humic Materials--

The DW concentrates produced by XAD-2 resin extraction of the RO brine contained a significantly greater amount of organic material than those produced by solvent extraction of RO brine. In Table 7, three digit code names ending in "C" designate concentrates produced by solvent extraction of the RO brine while those ending in "X" correspond to subsequent XAD-2 resin extraction of the RO brine. Comparison of the concentration values for corresponding concentrate pairs illustrates the higher efficiency of XAD-2 resin extraction, especially since solvent extraction was performed on the RO brine prior to XAD-2 resin extraction. The experimental observations indicate that much of the additional organic material recovered by XAD-2 resin extraction was humic-related substance. These observations indicating the presence of large amounts of humic materials include the following:

- The color (aqueous, high pH) was amber-brown and the UV spectrum showed a very broad maximum in the 250 nm region
- Aqueous solubility was greatly enhanced at high pH
- Extraction efficiency from aqueous media at low pH with methylene chloride was poor resulting in low total recoveries
- GC-MS analysis of the derivatized acid fraction always resulted in a broad, late-eluting range of unresolved components generally attributable to oligomeric humic materials
- GC injections of this fraction always resulted in a significant amount of a dark brown residue of pyrolized, nonvolatile material in the quartz injector liner.

The effectiveness (greater than 90 percent at low pH) of XAD-2 resin in removing humic and fulvic acids from dilute aqueous solution has been demonstrated by Mantoura and Riley who show this resin to have a capacity exceeding 20 mg/gm before the onset of recovery degradation (9).

Detection of Special Interest Compounds

The numbers of "Special Compounds" shown for the concentrates in Tables 7 and 8 roughly correlate with the total number of compounds detected, as might be expected. One-half to two-thirds of the detections enumerated under the "Specific Search" heading would not have occurred without the computerized GC-MS data searching which was developed for this work and is described in Section 5 and Appendix A. "Specific Search" detection instances in Tables 9 and 10 with RS values 1.0 or less generally were not detectable without the use of this special GC-MS data searching software. Note that many of the compounds on the "Specific Search" list (these 53 compounds are listed in Table 4) are also members of the other two lists that are tabulated. Thus, there is appreciable redundancy in the numbers shown in these three columns in Tables 7 and 8.

Tables of Identified Compounds

Description of the Tables--

Identified compounds for the DW and AWT concentrates are listed in Tables 9 and 10, respectively, and as a combined DW and AWT listing in Table 11. These tables show in which concentrate each of the compounds were identified by indicating the RS value for the GC-MS peak. The compounds are arranged in decreasing order of the largest RS value found for each compound. In addition, instances of detection which were judged to be attributable to the blank are designated with an asterisk in these tables. The criteria used to attribute detected compounds to the blank is described and discussed in this section under "Screening Compound Identification Results for the RO Process/Concentrate Production Blank".

Selection of Concentrates for Inclusion in the Combined Results Tables--

The computer software which produced the combined concentrate report tabulations (Tables 9 and 10 for DW and AWT, respectively) allowed the results of a maximum of 18 concentrates to be displayed in one table. Since there were only 16 AWT concentrates (Table 8) and 2 relevant blanks (concentrates V1C and X1C), it was not necessary to omit any of the AWT concentrates from that combined results table (Table 10). However, in the case of the DW concentrates (Table 7), there are 15 concentrates and 5 relevant blanks (concentrates V1C, V1X, T2B, X1C, and X1X). Thus, it was necessary to omit two concentrates from the combined DW results (Table 9), and the Miami II XAD and New Orleans II XAD concentrates (M2X and N2X, respectively, Table 7) were omitted since these two concentrates were heavily contaminated by XAD-2 resin bleed artifacts. For example, of the 204 neutral compounds identified in the M2X concentrate, 133 (65 percent) were attributable as artifacts due to XAD-2 resin bleed, and the corresponding result for concentrate N2X was 90 of 181 neutral compounds (50 percent) attributable as XAD-2 resin artifacts. For completeness, compound identification results for these two concentrates are presented in Volume 2, Appendix A.

The computer software which produced the DW plus AWT combined concentrate report tabulation (Table 11) allowed the results for a maximum of 27 concentrates to be displayed. With a total of 36 concentrates (16 AWT, 15 DW, and 5 "Blanks"; see Tables 7 and 8), it was necessary to exclude 9 of these concentrates from Table 11:

- The two solvent blanks, X1C and X1X, were excluded
- The two contaminated XAD DW samples, M2X and N2X, were excluded as for Table 9
- Concentrate L2M was chosed as representative of the Lake Tahoe II samples, thereby excluding concentrates L2P, L2N, and L2D (see Table 8)

- Concentrate C1M and C1N were chosen as representative of the Pomona I samples, thereby eliminating concentrate C1P
- The B1M and B1N concentrate results were combined as a new concentrate named B3C in the database.

Screening Compound Identification Results for the RO Process/Concentrate Production Blank--

The method of data correction for artifacts introduced during concentrate partitioning and sample analysis has been addressed in Section 5. In summary, this procedure effectively eliminated the possibility of introduction of concentrate partitioning artifacts into the computer-managed database.

Concentrate production from the sampled water was performed by other laboratories under separate contracts (see Section 4) and, thus, monitoring and characterization of artifacts due to concentrate production procedures was not under Battelle's direction. Because of this circumstance and also because the concentrates functioning as blanks for these processes were not available at the beginning of the research program, screening of artifacts due to the concentrate production process could not be performed prior to introduction of compound identification results into the computer-managed database. Thus, this blank screening has been performed manually after computer processing of the compound identification analysis results.

The blank concentrates--To allow some degree of control against reporting artifacts due to the concentrate production procedure, five concentrates were analyzed as blanks:

- V1C: Poplarville I Composite Concentrate (Table 1)
- V1X: Poplarville I XAD Concentrate (Table 1)
- X1C: Composite solvent extract blank (Table 3A, Appendix A)
- X1X: XAD-2 resin elution blank using ethanol (Table 3A, Appendix A)
- T2B: XAD-2 resin elution blank using diethyl ether (Table 3A, Appendix A).

Blank concentrate T2B corresponds as a simultaneous concentration production blank to concentrate T1Y, the only concentrate produced by direct adsorption/elution using XAD-2 resin (i.e., RO preconcentration was not used). Therefore, T2B is the only blank concentrate which corresponds uniquely to a sampling incident.

In screening the compound identification results for possible artifacts due to the concentrate production methodology, criteria based on RS values of GC-MS peaks (described below) were applied to Tables 9 and 10. The blank screening results obtained were added to Table 11.

Screening criteria for DW concentrates--XAD-2 resin bleed artifacts were identified in the T1Y, T1X, T4X, P2X, O2X, and S2X concentrates based both on the results of the T2B, V1X, and X1X blanks (shown in Table 9) and on experience with samples heavily contaminated with XAD-2 resin bleed artifacts.

(See, for example, the analysis results for concentrate M2X in Volume 2, Appendix A, Table 1A, and the discussion of the XAD-2 resin bleed artifact problem in Volume 3.) The main criterion for designation of identified compounds as XAD-2 artifacts was the compound class. The observed relative concentrations of these XAD-2 resin artifacts were consistent with the usual pattern. The absolute level of concentrate contamination, however, varied widely among the XAD-2 concentrates.

The results from concentrates V1C, V1X, X1C, and X1X were used to screen the compounds identified in the DW concentrates for artifacts attributable to sources other than XAD-2 resin bleed. In this case, the RS value was the main criterion used to judge whether a compound which was found in the blank concentrates, V1C, V1X, X1C, and X1X, should be disregarded when found in one of the DW concentrates. If, for a given compound, the RS value for detection in the blank was exceeded by the RS value for detection in a sample concentrate by 2.0 or more units (i.e., a factor of 10 difference in relative size of the GC-MS peak), then the sample concentrate detection was considered genuine (i.e., not an artifact). Since levels of artifacts introduced by RO processing and solvent and XAD-2 extraction of the RO brine might be expected to be independent of the volume of water sampled, the RS values used for this blank screening test should be those originally resulting from comparison of the GC-MS peaks with the internal standard according to Table 5. The RS values appearing in Table 9 were obtained by normalizing the original RS values to the "standard" 1514-liter sample volume using Equation 3 of Section 5. Thus, the RS values of Table 9 had to be converted before volume normalization so that the 2.0 RS value increment criterion could be applied. Because RS values span a logarithmic scale, this adjustment to the pre-normalized value involved only adding an appropriate constant to the RS values in Table 9. These constants were: V1C and V1X, 2.0; T4C and T4X, 1.1 (applied after the correction noted in Table 9); M2C, 0.4; N2C, 1.3; P2C and P2X, 1.2; O2C and O2X, 1.1; S2C and S2X, 1.8. Since the water volume for T1C and T1X was about the same as that taken as the "standard" volume, these two concentrates required no RS value adjustment before comparison to the blank RS values. In addition, the blanks, X1C, X1X, and T1Y, were considered to correspond to the "standard" 1514-liter sample; thus, no adjustment in RS values was made before blank screening comparisons.

Screening criterion for AWT concentrates--All of the AWT concentrates were prepared from approximately 400 gallons (1500 liters) which corresponds to the "standard" volume to which RS values were normalized. Thus, adjustments to RS values in Table 10 prior to application of the 2.0 RS value increment criterion was required only for the V1C concentrate RS value (2.0).

Results of artifact screening--For the DW results (Table 9), 119 compounds detected had 238 detection instances for XAD-2 produced concentrates classified as artifacts due to XAD-2 resin bleed. In addition, another 68 compounds detected in the 15 DW concentrates had 266 detection instances classified as concentrate production artifacts from sources other than XAD-2 resin. Thus, a total of 187 compounds with 504 detection instances have been designated as artifacts in Table 9. Since none of the AWT concentrates were prepared by XAD-2 extraction of the RO brine, only the compound identification results for the blank concentrates V1C and X1C were appropriate for screening artifacts in AWT concentrate results, and 274 detection instances of 65 compounds in Table 10 were thereby attributable to non-XAD-2 sources of contamination.

The results of screening the compound identifications for artifacts attributable to the concentrate production process should be considered tentative. The absence of results for analysis of replicate blank concentrates together with the unavailability of a definitive demonstration of the appropriateness of the blanks that were analyzed and reported here prevent assignment of high levels of confidence in some of the listings of Tables 9, 10, and 11. Indeed, compounds listed in these tables which were detected both at very low levels (generally at RS values of less than 2.0) and in isolated instances (i.e., detection occurred in only one or two concentrates) should be regarded as more tentative than others.

Some considerations which should have a bearing on the interpretation of the results of artifact screening in Tables 9, 10, and 11, include the following:

- Except for the XAD-2 artifacts, screening of most compounds was due to detection in concentrate V1C. Since this concentrate (as well as concentrate V1X) corresponds to a sampling of an extremely large volume of DW, many of the compounds detected and assumed to be artifacts may have been present in the water. Examples include the compounds pentachlorophenol, 2,4,6-trichlorophenol, p-cresol, 2,4,6-trichloroaniline, tributyl phosphate, benzthiazole, 2,6-di-t-butyl-p-benzoquinone, and dehydroabietic acid.
- There are many compounds in Tables 9, 10, and 11 for which the RS value criterion resulted in the classification of numerous, but not all, identifications as artifacts. For those compounds with RS values large enough not to be classified as an artifact, it is possible that the compound was actually present as an artifact at a higher than usual level. Of course, the greater the ratio for a given compound of detection instances classified as artifacts to those not so classified, the greater the probability may be that more of the detection instances should have been classified as artifacts.
- It is possible that all artifacts due to concentrate preparation were not detected in the five blank concentrates. Thus, compounds with molecular functionality closely related to a class of compounds generally designated as artifactual may also be artifacts. This possibility is particularly noteworthy in the case of fatty acids, fatty alcohols, and common plastizers, especially diesters of phthalic and alkanedioic acids.
- Most of the compounds detected in the blank concentrates (except for the XAD-2 artifacts and those clearly related to extraction solvent impurities) are ubiquitous in the

environment and, thus, even though detected in a blank concentrate, there remains a reasonable probability that these compounds were indeed present in the DW and AWT water samples. Again, fatty acids, fatty alcohols, and plasticizers, as well as polyglycol ethers, are primary chemical classifications for this consideration.

Use of the Molecular Weight Table

In order to determine whether a given compound was found in any of the DW and AWT concentrates, it was necessary to produce a listing of the identified compounds, ordered by molecular weight, which was correlated with Tables 9 and 10. The required listing is presented in Appendix D of this volume, and the structure and use of this listing and the significance of listed compounds which are not indicated as having been found in any of the concentrates are also discussed here.

Additional Listings of Compound Identification Results

Volume 2 contains the complete set of computer-printed tables for DW and AWT concentrates. Tables 9, 10, and 11 of Volume 1 which list the identified compounds for DW concentrates, AWT concentrates, and 24 selected DW and AWT concentrates, respectively, are, individually, the first parts of three-part tables. The second and third parts of these tables containing information not discussed in Volume 1 appear only in Volume 2. Four of the twelve available tables summarizing occurrences of functional groups appear in Volume 1. The computer-printed tables which appear in Volume 1 are also presented in Volume 2 in order to present the complete set of results in that Volume. The additional information provided by the complete set of listings is the following:

1. Identification status (confirmed or tentative) for all compounds identified in concentrates
2. Systematic names, molecular formulas and molecular weights of all identified compounds
3. Functional group information for each concentrate showing the total relative size values for each functional group on each of the two GC columns (SP1000 and SP2100).

The reader is referred to Appendix F which contains the Table of Contents and List of Tables for both Volume 2 and Volume 3.

Number of Identified Compounds

Tables 9, 10, and 11 list the following numbers of unique organic compounds:

Table 9 - 13 DW concentrates: 1091 compounds

Table 10 - 16 AWT concentrates: 991 compounds

Table 11 - 24 DW and AWT concentrates: 1423 compounds.

Compounds that were detected in one or more of the blank concentrates (V1C, V1X, X1C, X1X, and T2B) but not in any other concentrate are not included in the above totals; there are 87, 25, and 49 of these compounds in Tables 9, 10 and 11, respectively. Compounds for which more than half of the entries in a given table are attributed to the blank are also not included in these totals; 138, 58, and 143 such compounds were found in Tables 9, 10, and 11, respectively. Tentatively identified compounds which appear in these three tables that were later confirmed to be absent have a line drawn through them to indicate that status. There are 21, 32, and 26 such corrections in Tables 9, 10, and 11, respectively.

Results of Analysis of Blank Concentrates

The Poplarville, Mississippi DW concentrates, V1C and V1X, resulted in the largest numbers of compounds among the 5 concentrates analyzed that served as blanks. These two concentrates were prepared from the same RO brine with the V1C concentrate being produced by solvent extraction of the RO brine and the V1X concentrate being produced by re-extraction of this same RO brine using XAD-2 resin, as per Table 1 and the discussion in Section 4, Concentrate Production. The results of the V1X concentrate provided only additional data on the nature of XAD-2 resin bleed artifacts since 133 of the 158 compounds identified (84 percent) qualify as such. Of the 55 largest GC peaks (RS values 3.0 or greater) for both of these concentrates, 52 were found exclusively in V1X, and all but two of those 52 compounds, which were both phthalates, were XAD-2 resin bleed artifacts. Except for the small volume samples associated with Jefferson Parrish (Volume 3), the V1X concentrate was the most heavily contaminated by XAD-2 resin bleed materials of all the concentrates analyzed. Only 9 of the 208 different compounds were identified in both the V1C and V1X concentrates. This surprising agreement disparity between the results of these two concentrates is probably the result of both the dominance of the XAD-2 resin artifacts in concentrate V1X and the extremely low level of organic contamination of the water. For example, only two compounds of concentrate V1C have RS values greater than 2.0, none have RS values greater than 3.0, and 60 percent of the identifications have RS values of 0.0 or -1.0. Only 59 compounds were identified in concentrate V1C. The predominant species in concentrate V1C were fatty acids (9 compounds), fatty acid methyl esters (9 compounds), plasticizers (6 phthalates and 1 adipate), resin acids (3 compounds), and alcohols (8 compounds).

Blank concentrates X1C and X1X were intended to reveal artifacts other than those associated with the RO apparatus. Concentrate X1C was a composite of K-D distilled solvent of the type used for RO brine extraction while X1X was K-D distilled ethanol which had been used to elute a blank column containing XAD-2 resin. Only 50 compounds were identified in concentrate X1C, and, as expected, these compounds were predominantly solvents: chloroalkanes, alcohols, and ketones. Phthalates and other plasticizers were identified at lower levels, and fewer were found than for other concentrates. However, fatty acids (8 compounds) were identified with RS values in the 2.0 to 5.0 range.

Similarly to concentrate V1X, the X1X concentrate predominantly contained species ascribable as XAD-2 resin bleed artifacts (about 30 of 58 compounds). In contrast, however, these artifacts were found at substantially lower concentration for concentrate X1X than for concentrate V1X, above. Only nine compounds were found with RS values greater than 3 and only two of these compounds had RS values of 4.2. Aside from the XAD-2 artifacts, the predominant species were fatty acids, alcohols, and ethyl esters (presumably produced by reaction with the ethanol solvent) and ketones.

Concentrate T2B was the only blank concentrate which was processed as a blank for a specific concentrate, corresponding to concentrate T1Y. Concentrate T2B was a blank elution of XAD-2 resin using diethyl ether eluent. The T2B concentrate contained few organic compounds and most of the identified compounds are expected for an XAD-2 resin elution. Only 13 of the 99 identified compounds had RS values greater than 3.0. Moreover, 56 of the 130 identifications in the eight fraction analyses were assigned the RS value of 1; however, many of these peaks were actually smaller than this size range. Most of the aromatic or partially reduced aromatic materials identified are probably XAD-2 resin bleed artifacts. All of these artifacts, however, have very low RS values of 2 or 1. In addition, only 21 of the 99 compounds shown in Table 9 for T2B have been classified as XAD-2 resin bleed artifacts. The T2B concentrate contained the lowest levels of XAD-2 resin bleed artifacts of the XAD concentrates that were analyzed. High levels of benzoic acid and methyl benzoate (RS values 5.0 and 7.0, respectively) were found. While benzoic acid was often found at relatively high levels in XAD concentrates, the concentrations did not correlate with the much more predominant artifacts, the alkyl and alkenyl arenes. In addition, benzoic acid was always found in the corresponding solvent extract concentrate. In contrast, methyl benzoate was identified only in concentrate T1Y (for which T2B is the process blank). High levels of these two compounds in T2B is, therefore, considered to be an isolated instance. Predominantly, the non-XAD artifact compounds included alcohols, ketones, fatty acids, esters (both alkyl and aryl, mostly methyl), and diester plasticizers.

DISCUSSION OF DW CONCENTRATE ANALYSIS RESULTS

Summaries of the Results for Each Sampling

Poplarville, Mississippi, March 2, 1979--
The analysis results for the two Poplarville concentrates, V1C and V1X, which function as concentrate production method blanks in this work but, nevertheless, were prepared from finished DW are presented in this section under Results of Analysis of Blank Concentrates.

Cincinnati, Ohio, October 17, 1978--
T1C: combined solvent extract of RO brine--There are three main features of the T1C concentrate results that distinguish this DW concentrate from all the others:

1. Sixteen species of alkylated pyridines were identified in the fraction containing the extracted bases. Most of these compounds were found at moderately low concentrations (RS values 1.0 to 3.0). Compounds of this functionality have rarely been identified in DW concentrates from other samplings.

2. Dichloroaniline, trichloroaniline, and tetrachloroaniline were identified in the aromatic fraction. Compared to the other constituents in this fraction, the amount of dichloroaniline (RS value 3) was surprising. Chloroanilines were not often encountered in other concentrates at levels this high. Both 2-chloroaniline and pentachloroaniline are compounds for which the data were specifically searched (Table 4). However, neither of those two members of the chloroaniline series were detectable by specific search of the T1C concentrate data.

3. Relatively high levels of chloroalkanes and chloroalkenes were identified in the aromatic fraction. In particular, the 1,2,3-trichloropropane component was present at high concentration (RS value 6.0). Usually, aromatic materials constitute the bulk of the identified compounds in this fraction. However, in the case of concentrate T1C, C_3 halo-hydrocarbons and haloforms are the principal constituents. In addition to this very large component, 1,1,2-trichloropropane, 1,1,2-trichloropropene, 1,1,3-trichloropropene, two isomers of bromodichloropropane, bromoform, dibromochloromethane, and bromodichloromethane were also identified. All of these halohydrocarbons should have been predominantly in the alkane fraction which was not analyzed by GC-MS. Indeed, the residue weight results suggests that the presence of these compounds in the aromatic fraction is overlap from unusually high levels in the alkane fraction, since the alkane fraction contained about eight times as much material as the aromatic fraction. For most DW and AWT concentrates, the alkane fraction contained less or a comparable amount of material compared to the aromatic fraction. Thirteen of seventeen compounds (76 percent) identified in the aromatic fraction contained halogen. The most probable conclusion is that either the sampled DW was unusually contaminated with halogenated solvents or that the solvent used to extract the RO brine was contaminated with these halogenated materials.

The compounds identified in the derivatized acid fraction were not surprising. Fatty acids from C_5 to C_{15} were present at high relative amounts with a significant absence of unsaturated members of the series. Methylethylmaleic acid and dimethylmaleic acid were among the largest peaks. Salicylic, clofibric, and benzoic acids were detected as expected water re-use indicators. The aromatic acids detected include a number of alkylated benzoic acids, phenylacetic acids, and phenoxyacetic acids (including 2,4-D and 2,4,5-T). The presence of 2-aminobenzoic acid and 3,6-dichloro-2-methoxybenzoic acid (the herbacide, dicamba) may be noteworthy. The dichloroacetic, trichloropropenoic, and dichlorobutenoic acids detected may indicate the presence of other polychloro carboxylic acids which are not recovered due to high acidity (i.e., trichloroacetic acid). The only phenols identified were three compounds which are on the specific search list: phenol, 4-chlorophenol, and pentachlorophenol.

The medium polarity fraction contained, in addition to the large number of pyridine compounds noted above, the following nitrogen-containing species: phenyl acrolein, a C_6 amide, N-acetyl morpholine, phenyl acetonitrile, nicotine, and five quinoline isomers.

One of the largest components of the high-polarity fraction was 1,3,5-trimethyltriazine-2,4,6-trione (Trimethylisocyonurate), frequently detected at moderately high levels in concentrates from DW with sources similar to the Ohio River. A variety of ketones, alcohols, alcohol-ethers, phthalic diesters and alkane-dioic diesters have been identified in the high polarity fraction and are probably attributable to the RO process blank. N,N'-dimethyl urea, triethyl phosphate, tributyl phosphate and N-acetyl morpholine (the latter also identified in the medium polarity fraction) may be noteworthy identifications in this fraction.

T1X: XAD-2 extract of RO brine--A smaller portion, 4 percent instead of 10 percent, of the total T1X concentrate was partitioned into fractions for GC-MS analysis; thus, all potential detection limits for this analysis were higher by a factor of 2.5. In agreement with the Project Officer, it was judged not cost effective to repeat analysis on this sample. Inspection of the GC-MS chromatograms of the fractions revealed excellent signal to noise with regard to detection of the internal standards. Thus, the relatively smaller number of identifications for concentrate T1X compared to concentrate T1C (66 versus 140, respectively) are ascribable to the nature of the sample rather than to the amount of concentrate which was analyzed. RS values of identified components were adjusted to account for this factor of 2.5.

Comparison of the identification results for concentrates T1C and T1X clearly indicates that the solvent extraction of the RO brine (T1C) which preceded the XAD extraction of that same RO brine (T1X) was very effective in removing most of the less polar components. This conclusion is easily verified by comparing RS values of compounds found in both concentrates (Table 9). Generally, only the alcohols, ketones, and acids are reported in concentrate T1X with RS values as high or higher than the corresponding values for T1C. Furthermore, Table 7 indicates that only 12 percent of the concentrate was recovered into fractions and that more than 90 percent of that recovered material was in the acid fraction. Thus, concentrate T1X consisted principally of humic-related materials which were not solvent extractable from the RO brine.

The acid fraction contained some interesting chlorinated acids: 2,4-dichlorobenzoic acid, tetrachloroterephthalic acid (probably from the pre-emergence herbicide, chlorthal-dimethyl which has a half-life towards hydrolysis to the free acid of 100 days in soil), trichloropropenoic acid, dichloroacetic acid, 2,2-dichloropropanoic acid (the herbicide, dalapon) and 2,2-dichlorobutanoic acid. Identification of N-hydroxyphthalimide, a hydroxamic acid, may be noteworthy. Benzoic acid and methylethylmaleic acid were the largest components of the acid fraction. However, results from the blank T1Y, indicate most of the benzoic acid is probably an artifact. The often encountered salicylic, benzeneacetic, phthalic, and dimethylmaleic acids were also identified in the acid fraction.

Concentrate T1X had distinctly fewer aromatic organic compounds than the other DW concentrates. No residue weight was detected after correction for the blank, and 3 of the 4 compounds found (naphthalene, 2-methylnaphthalene and phenanthrene) may be attributable as XAD-2 resin bleed artifacts. Few noteworthy compounds were detected in the other two fractions (medium and high polarity). This result is consistent for the very low relative recoveries shown in Table 7. Phenol (possibly an XAD-2 artifact in this case), isophorone and the relatively high polarity compounds, benzaldehyde (at least partially attributable to XAD-2 resin bleed) and nicotine may be of some interest.

T1Y: direct XAD-2 extraction with diethyl ether elution--Concentrate T1Y is unique among all the concentrates analyzed since it is the only one produced without any use of RO pre-concentration. This concentrate contained an unusual set of industrially-related organic compounds of which many were halogen substituted. Of the 211 compounds identified (Table 7), 87 (41 percent) contained one or more halogen atoms. For the aromatic fraction, the percent of halogen containing compounds is 84 percent with 18 percent of the identifications containing one or more bromine atoms. Chlorine and bromine were the only halogen substituents found. The total of 17 specific search compounds found in the T1Y data are listed in Table 17. This concentrate contains the highest number of identifications of specific search compounds of the DW concentrates and is exceeded by only one of the AWT concentrates (Tables 7 and 8). Moreover, of these 17 specific search compounds, 12 (71 percent) contained chlorine. The number of identified compounds (24) on the "Chemical Indicators of Industrial Pollution" list was the highest number identified in any concentrate. In addition, the number (13) of Consent Decree compounds was equalled only by concentrate T4C and exceeded only by concentrate N2C (15 compounds). A further indication of the high levels of halogenated compounds was that 140 (64 percent) of the unidentified mass spectra of GC-MS peaks showed the presence of one or more halogen atoms, and 53 percent of these unidentified mass spectra were from components in the aromatic fraction.

The level of contamination of the source water by haloforms and halogenated industrial solvents is actually greater than indicated by the results in Table 9. Analysis of the unpartitioned concentrate showed that the dominant constituents of the concentrate were CH_2ClBr, $CHCl_2Br$, $CHClBr_2$, bromo and chloro ethers, and other halo-hydrocarbons. These compounds would be predominantly recovered in the alkane fraction which was not analyzed by GC-MS, and detection in the aromatic fraction is due to overlap between these two silica gel elutions. Another observation for which concentrate T1Y was unique among the DW and AWT concentrates was a very pronounced late eluting range of poorly separated sample components in the high polarity fraction.

Another observation which distinguished the partitioned fractions of concentrate T1Y from most of the others analyzed is the absence of sample components which are present at significantly higher concentration than the majority of the other sample components. None of the GC-MS chromatograms for the partitioned fractions showed this often observed "tree stump" effect. In fact, the number of sample components and their relative concentrations were distributed among the various fractions in an almost optimal fashion for the analytical scheme. As noted above, however, there were "tree stump" components in the GC-MS chromatograms of the unpartitioned concentrate. These dominant components partitioned into the alkane fraction which was not analyzed by GC-MS.

The broad range of interesting and possibly significant compounds identified in concentrate T1Y is too lengthy to list as individual species. The following is a short summary of the more interesting types of compounds found:

- Phenols - 6 halophenols plus phenols
- Acids - chloro C_2, C_3, and C_4; numerous chlorobenzoic acids
- Herbicides and pesticides - 2,4,5-T, tetrachloroterephthalic (indicator of chlorthal-dimethyl), lindane and 2,4-D methyl and ethyl esters
- Halo/nitro aromatics - 18 halobenzenes and naphthalenes, 4 nitro benzenes, 4 chloro nitro benzenes, 3 chloro anilines, and PCBs (Cl_3 and Cl_4)
- Re-use indicators - clofibric acid, salicylic acid
- Other halo compounds - 5 chloro butenes and butadienes (including hexachloro), tetrachloropropane, 3 halo ethers.

Concentrate T1Y contained few XAD-2 resin bleed artifacts with only 21 of 243 identified compounds classified as such. This result is consistent with those for concentrates T1Y and T1X which used the same batch of carefully prepared XAD-2 resin.

Comparison of concentrates T1C, T1X, and T1Y--The water from which these three concentrates were derived was drinking water obtained during the period of October 16, 17 and 18, 1978. The water was sampled directly from a tap at the US EPA/HERL Laboratory in Cincinnati, Ohio. The sampled water was split into two streams of equal flow with each stream contributing a 1460-liter (387-gallon) sample. One stream was acidified to pH 2 with a metered flow of 6 N hydrochloric acid and immediately passed through an XAD-2 column. Subsequent elution with diethyl ether followed by volume reduction produced the T1Y concentrate. The other stream was used to fill a reservoir for the RO apparatus. Treatment of the RO brine by solvent extraction produced the T1C concentrate, while subsequent XAD-2 extraction of the RO brine produced the T1X concentrate (see Appendix E). Corrections in Table 9 for compounds which may have originated from the concentrate production method and which are based on the blank concentrates V1C, V1X, X1C, and X1X may be less valid for these three Cincinnati concentrates than for the other DW and AWT concentrates. Note, however, that blank T2B does correspond directly to concentrates T1X and T1Y with respect to artifacts due to the XAD-2 resin.

Focusing on a comparison of the residue weight results and compound identification results in Table 7 for concentrate T1Y and the composited values for concentrates T1C and T1X (hereafter referred to as T1C/T1X) reveals some interesting observations. If the process of reverse osmosis followed by solvent and then XAD-2 extraction of the RO brines (used for T1C and T1X) recovered organic materials equivalently to the process of direct XAD-2 adsorption/diethyl ether elution (used for T1Y), then the values for residue weight analysis in Table 9 ought to be comparable for T1Y and the composite T1C/T1X. Indeed, the amounts of material in the concentrates (expressed as "Concentration, μg/l") are essentially identical, at 540 and 527 μg/l for T1C/T1X and T1Y, respectively. However, comparison of the distribution of material in the recovered fractions (Table 7) and the numbers and identities of the identified compounds (Tables 7 and 9, respectively) shows substantial differences between T1Y and T1C/T1X.

Overall, the organic material of T1Y was recovered nearly twice as effectively through the partitioning scheme (Figure 4) as that of T1C/T1X (41 percent versus 23 percent, respectively). Enhancement (expressed as a percentage increase above T1C/T1X for T1Y) of recovery of concentrate material into the partitioned fractions was seen for all except the alkane fraction: acid, 35 percent; alkane, -22 percent (not shown in Table 7); aromatic, ~1800 percent (not calculable from Table 7, due to rounding); medium polarity, 130 percent; high polarity, 190 percent. In addition, T1X concentrate was a distinctly darker brown color than the T1Y concentrate. Optical densities were not measured, but if one assumes the brown color to be due principally to humic-related material in both concentrates, then T1X probably contained more than T1Y by a factor of 2 to 5.

There were more organic compounds identified in T1Y than in T1C/T1X. Enumeration of the listings of Table 9 shows that 154 compounds were identified in T1Y but not in T1C/T1X. Thus, only 55 of the 211 compounds (26 percent) identified in T1Y were also detected in T1C/T1X. There were 117 compounds identified in T1C/T1X but not in T1Y. For some of these compounds, a chemical explanation is readily apparent. The large number of nitrogen bases (23 compounds, mostly alkylated pyridines and quinolines or related species) detected in T1C and noted in the discussion above for that concentrate, undoubtedly were unretained by the XAD-2 resin since at pH 2 these compounds would be in the form of the ionic conjugate acids. Of the 97 other compounds detected in T1C/T1X but not T1Y, 80 (81 percent) had molecular functionality which would enhance water solubility and, thus, decrease recovery effectiveness by XAD-2 resin: 33 compounds were alcohols or poly glycol ether/alcohols; 16 compounds were low molecular weight ketones; 11 compounds were fatty or aromatic carboxylic acids; 12 compounds were relatively strong acids (chloro, keto, or hydroxy substituted or dicarboxylic); and 8 neutral compounds had exceptional polarity (i.e., amides, ureas, polar substituted esters or low molecular weight diesters). Only 17 of the 109 compounds do not have a polar molecular functionality reason for poor recovery by XAD-2, and 9 of these compounds may actually be RO process artifacts (3 plasticizers and 6 possible solvent impurity species).

Many of the 154 compounds identified in concentrate T1Y but not in T1C/T1X can be classified as the most hydrophobic/lipophilic materials among those identified. There are few acids and alcohols among this list (chlorobenzoic acids and halo phenols are exceptions). Most of the 154 compounds are low polarity aromatic compounds or have moderate polarity such as fatty acid methyl esters and ethers. Reinforcing these observations is the result that, for polar or moderately polar compounds found in both T1Y and T1C/T1X, the RS values for detection in T1Y are less (sometimes substantially) than those for detection in T1C/T1X. Moreover, the opposite is often true for polar compounds detected in both T1Y and T1C/T1X. Many of the compounds which are exception to the above observation are attributable as concentrate production method artifacts.

Since this set of concentrates are the only ones for which direct comparison of RO-based concentration technique (T1C/T1X) can be compared with the direct adsorption/elution technique (T1Y), it is not possible to propose a definitive explanation for the results. However, the following seems to be consistent with both the observations and chemical expectations:

- Poor recovery of small and moderate sized apolar species (i.e., substituted benzenes) is due to permeation by these species of the RO membranes. In aqueous solution, these molecules exist as non-solvated species in a hydrophobic "shell" so that their sizes are not enlarged above the molecular size by a tightly associated solvation sphere. Thus, diffusion of these materials into membrane pores requires no de-solvation energy, and, indeed, this process is thermodynamically driven by the "hydrophobic energy" released when water molecules in the solvent shell become fully solvated in the bulk solvent. Of course, this thermodynamic driving force would have to be repaid for the hydrophobic species to appear in the permeate water, but only after the membrane capacity for these apolar materials was exceeded, and that point may often not be reached for DW samples. XAD-2 resin would, of course, have very high capacities for these apolar species.
- Highly polar, especially oxygen and nitrogen containing species, and/or ionized species would have a substantially larger size in aqueous solution than their actual molecular sizes due to tightly bound, multiple layered solvation spheres. Thus, these species should be retained well by the RO membranes, and the nonionic and ionization suppressable species can, of course, be recovered by solvent extraction or XAD-2 extraction of the RO brines. In contrast, due to the enhanced water solubility of these polar materials, they would not be retained as well by the XAD-2 resin as more apolar species.
- Macromolecular hydrophilic materials such as humic-related substances and poly glycols would be very effectively retained by the RO membranes. Solvent extraction of the RO brines effectively recovers the poly glycols but not the

humic-related materials. However, as pointed out above, the analysis results definitely indicate that the humic-related material is recovered better by XAD-2 extraction of the RO brine than by XAD-2 extraction of the water directly. Since the volume of the RO brine was about 0.05 percent of the starting water (see Appendix E), the k' values for the humic-related material may not be exceeded in XAD-2 resin extraction of RO brine (approximately 4 bed volumes of RO brine passed through the column) whereas they may be considerably exceeded in the direct XAD-2 extraction (approximately 8000 bed volumes passed through the column).

- The essentially equal recoveries into T1Y and T1C/T1X from the starting water (Table 7) is apparently coincidental: the recovery losses of the direct XAD-2 resin adsorption technique for the more water soluble materials including humic-related substances are approximately equal to the recovery losses of the RO membrane for apolar materials.

In summary, the results definitely indicate that direct XAD-2 extraction of DW is superior to RO pre-concentration methods when the target compounds are relatively apolar organic materials of the type usually encountered as organic industrial effluents. The opposite is true for strong acids, alcohols, humic-related material and other highly water soluble and/or macromolecular organic materials.

Cincinnati, Ohio, January 14, 1980--

T4C: combined solvent extract of RO brine--Residue weight analysis of concentrate T4C (Table 7) yielded a value of 115 μg/l as the concentration in the original water which the organic material recovered into this concentrate represents. This value is lower than corresponding values for all other DW concentrates except for Seattle, Washington (37 μg/l) and Poplarville, Mississippi (0.6 μg/l) which serves as the blank in this work. For comparison, the prior sampling (October 17, 1978) of Cincinnati DW gave a solvent extract of RO brine concentrate representing 143 μg/l of organic material in the original water (Table 7).

Only 36 percent of the original concentrate material was recovered in the analyzed fractions, and 71 percent of this recovered material was in the acid fraction. This low overall recovery (of all DW solvent extract concentrates, only that for Poplarville was lower) and relatively high percentage of recovered acids is indicative of humic-related species as the predominant organic material present. This indication is confirmed by the presence of the usual range of unresolved GC-MS peaks in the chromatograms of the unpartitioned concentrate and the acid fraction.

Although the acid fraction contained substantially more material than any other analyzed fraction, there was no highly dominant set of compounds in this fraction or any other fractions as is often the case for phthalates, polyglycols or fatty acids. Dimethylmaleic acid and ethylmethylmaleic acid were among the components present in the highest concentrations in the acid fraction. However, RS values for thses two compounds were about average as compared to other DW concentrates (entries 14 and 7, Table 9, respectively). In addition, about as many aliphatic and unsaturated carboxylic acids were present as phenyl substituted carboxylic acids, with the aromatic species at slightly lower concentrations.

There were nine specific search compounds identified in the acid fraction (concentration, ng/l, shown in parentheses): 4-chlorophenol (46), 2,4-D (44), 2,4,6-trichlorophenol (31), phenol (18), 2,4,5-T (4.7), 4-methylphenol (3.0), 2,4-dimethylphenol (2.8), pentachlorophenol (2.6), and 2,4-dichlorophenol (2.5). These nine acidic compounds were found with higher RS values than all of the non-acidic specific search compounds found (concentration, μg/l, shown in parentheses): nitrobenzene (3.3), 2-chloroaniline (1.6), 2-chlorotoluene (1.6), styrene (0.8), 1,4-dichlorobenzene (0.4), 2-methylstyrene (0.1), and fluoranthene (0.1). These sixteen specific search compounds were second in number only to concentrate T1Y among the DW concentrates.

The usual water reuse indicators have also been found: clofibric acid, salicylic acid and caffeine at comparatively high concentrations and nicotine at substantially lower concentration. A number of phenolic antioxidants, probably originating as food preservatives, were also identified.

A few compounds which may be indicative of contamination from industrial sources are noteworthy: pyridine and five alkyl pyridine isomers; N,N-dimethyltoluyl amine; dimethylformamide; nitrobenzene, nitrotoluene and dinitrotoluene; three organophosphates (triethyl, tributyl and tris-2-chloroethyl); a variety of chlorinated propanes, propenes, ethanes, and ethylenes; and 2-chloroaniline, 2,4-dichloroaniline and 2,4,6-trichloroaniline. Also found at relatively high concentration was 1,3,5-trimethyl-1,3,5-triazine-2,4,6-trione (trimethylcyanurate). This compound (entry 53, Table 9) was identified in three other DW concentrates: T1C and T1Y (Cincinnati) and N2C (New Orleans). It has also been identified in a number of the Cincinnati small-volume samples described in Volume 3.

T4X: XAD-2 resin extract of RO brine--Concentrate T4X contained XAD-2 resin bleed artifacts in amounts which, relative to the other XAD-type concentrates analyzed, can be described as moderately high. Of the 181 compounds listed for T4X in Table 9, 56 have been classified as XAD-2 resin bleed artifacts and 12 have been attributed as concentrate production artifacts from other sources. Thus, the net number of identifications for this concentrate is 113. The lower overall recovery of material into the analyzed fractions, as compared to the solvent extracted concentrate, T4C, is consistent with similar results for the other pairs of DW concentrates (Table 7).

Of the 48 compounds identified in the aromatic fraction, only 2 have not been classified as XAD-2 artifacts. Undoubtedly, the high XAD-2 artifact background prevented identification of some apolar species present at low concentrations. Most of the apolar compounds in the RO brine should have been recovered in the solvent extract concentrate, T4C, and, thus, little information was lost due to the XAD-2 artifact interference.

The acid fraction contained a distribution of fatty and aromatic carboxylic acids plus a relatively large number of strong acids (dicarboxylics and chloro or keto substituted). Water reuse indicators in the acid fraction included salicylic acid, saccharin, and ethosuximide. The herbicide, dicamba and tetrachloroterephthalic acid (degradation product of the herbicide chlorthal-dimethyl), were also detected. Phenol, p-cresol and 2,4-dimethylphenol were the only phenolics found, and the latter two were at very low concentrations.

Noteworthy compounds found in the medium polarity fraction include the following nitrogen containing compounds: pyridine, aniline, 2-chloroaniline, dichloroaniline, diphenylamine, benzylamine, N,N-dimethylbenzylamine, caffeine, nicotine, N-methyl-γ-butyrolactam, and diethylformamide.

The methanol silica gel eluate, Fraction 7, contained poly glycol materials as the predominant species. Three homologous series of these compounds were identified as the major constituents of the fraction. Noteworthy compounds identified included DMF, caffeine, acetanilide, 3-acetylaniline, N-methyl-γ-butyrolactam and isophorone.

Comparison of concentrates T4C and T4X--The T4C and T4X concentrates were prepared from about 7,570 liters (2000 gallons) of finished drinking water. The organic material was pre-concentrated by reverse osmosis (RO) using cellulose acetate and DuPont Permasep® nylon hollow fiber RO units as described in Section 4. The water was sampled at the Cincinnati, Ohio waterworks on January 14, 1980, and was taken from the process stream at a point just prior to treatment by contact with a one million gallon per day granular activated carbon (GAC) unit. A number of relatively small volume samples (corresponding to 10 to 30 liters) were taken at various stages of the RO processing scheme. Analysis results for these 13 small volume samples, associated with GAC contactor "A", are presented and discussed in Volume 3. Although 7,570 liters of DW were RO processed by GSRI, 70 percent instead of 100 percent of the RO brine produced was used by GSRI to generate concentrates T4C and T4X. This information was not conveyed to Battelle until analysis work was completed. Thus, the GC-MS analyzed portion of the material recovered from the sampled DW was 7 percent rather than the usual 10 percent. The water volume shown in Table 7 for concentrates T4C and T4X is 70 percent of that volume actually sampled since that is the volume of water actually corresponding to the results obtained for these two concentrates.

As usual, the XAD-2 resin produced concentrate, T4X, contained considerably more organic material than the composite solvent extraction concentrate, T4C, with 745 μg/l and 115 μg/l for T4X and T4C, respectively. The material left in the RO brine after extraction of the T4C concentrate was, as usual, relatively more polar. Thus, the T4X concentrate was not as well recovered into the partitioned fractions as the T4C concentrate: 23 percent for T4X compared to 11 percent for T4C. The higher range of polarities expected in the T4X concentrate also accounts for the greater portion of recovered material that the acidic fraction represents: 91 percent for T4X versus 72 percent for T4C.

It is also noteworthy, in comparing the T4C and T4X results, that fewer specific search compounds were found in T4X (seven compounds) than in T4C (sixteen compounds). Five of the seven specific search compounds found in T4X were also found in T4C: phenol, 4-methylphenol, 2,4-dimethylphenol, 2-chloroaniline, and fluoranthene. In each case, the quantitative results for the two concentrates agreed within a factor of three.

Comparing the acid fractions of concentrates T4C and T4X, the following observations are noteworthy:

- T4X contains stronger acids. For example, dichloroacetic acid, three chlorinated acrylic acid isomers, dichloropropionic acid and two isomers of dichlorocrotonic acid were found only in concentrate T4X. In addition, three dicarboxylic acids (phthalic, suberic and sebacic) were found only in T4X while a fourth (azelaic) was found at three to five times higher concentration in T4X than in T4C.
- The strong acid herbicide 2-methoxy-3,6-dichlorobenzoic acid (dicamba) and the degradation product of the herbicide chlorthal-dimethyl, tetrachloroterephthalic acid (chlorthal) were found in T4X. Chlorthal was not found in T4C, and dicamba was found in both concentrates but at substantially higher concentration (more than one order of magnitude) in T4X than in T4C.
- Saccharin and ethosuximide, both relatively strong acids, were found in T4X but not T4C.
- The phenoxy herbicides (2,4-D and 2,4,5-T), clofibric acid and four chlorinated phenols were found in T4C but not T4X.
- Both concentrates contained about equal amounts of salicylic acid and the usually encountered maleic acids.
- The T4X acid fraction chromatograms displayed a more distinct chromatographic profile of humic material than the corresponding T4C chromatograms. This result is consistent with all other solvent extracted and XAD-2 extracted DW concentrate pairs analyzed.

Miami, Florida, February 3, 1976--

M2C: combined solvent extract of RO brine--There are four main features which distinguished concentrate M2C:

1. The concentrate contained a relatively higher portion of humic-related materials than all of the other drinking water concentrates prepared by solvent extraction of RO brine.
2. There was a relatively large number of halogenated hydrocarbons present.

3. A number of sample components were present which clearly must originate from waste waters (water re-use indicators).

4. Di-n-butylphthalate was present at very high (and probably anomalous) levels.

Very prominent in the RGCs of the methylated acid fraction of M2C concentrate was the typical large, broad profile of unresolved middle to late eluting material which is characteristic of samples containing a high percentage of humic-related material. In addition, of the material recovered into the five fractions, 77 percent was in the acid fraction. This predominance of material in the acid fraction was not exceeded by any DW solvent extract type concentrates. The Cincinnati (T4C) and Ottumwa (O2C) concentrates were second and third at 72 percent and 68 percent, respectively.

The aromatic fraction contained an unusually large amount of halogenated material with 65 percent of the compounds identified in this fraction containing halogen. Tetrachloroaniline, bromoform, dibromochloromethane, chlorocyclohexane, bromocyclohexane, and iodocyclohexane, five chlorinated benzenes and 12 chlorinated hydrocarbons (C_2 to C_5) were identified in the aromatic fraction.

In the acid fraction, amobarbital, pentobarbital, clofibric acid and salicylic acid have been identified. These materials probably arise from wastewater sources since these compounds are all drugs or drug metabolites. All of these materials were found at surprisingly high levels considering the source of the Miami DW is groundwater.

It is readily apparent from the chromatograms of the unpartitioned concentrate that di-n-butylphthalate is the predominant constituent of the material in concentrate M2C. Based on the unpartitioned sample chromatograms, this n-butylphthalate component represented between 10 and 20 percent of the total GC-MS peak area. Since much of the ion current under the dibutylphthalate peaks probably saturated the signal electronics, the amount of this compound may actually be greater. Since many underivatized acids and humic-related materials undoubtedly did not elute in these unpartitioned chromatograms, it is not possible to approximate what percentage of the concentrate this di-n-butylphthalate represents. Similar concentrations of di-n-butylphthalate were observed in the Philadelphia and New Orleans solvent extract concentrates (P2C and N2C). Since all three concentrates were prepared about the same time (January 14, 1976 to February 3, 1976), the most reasonable explanation for the high levels of butylphthalate is that some change in the concentrate production procedure had occurred or contaminated extraction solvent was used over that short period of time. In addition, the XAD-2 extracts of RO brine for these cities (M2X, N2X, and P2X) contained either moderate amounts of dibutylphthalate or none at all. Thus, the artifact was probably not introduced during RO processing, but rather at or after the RO brine extraction sequence. There is no evidence to suggest that these phthalate components are not artifacts since other plasticizers were not present at even close to comparable levels.

Six compounds on the specific search list were found: phenol, 2,4,6-trichlorophenol, o-chlorotoluene, p-dichlorobenzene, 1,2,4-trichlorobenzene, and fluoranthene (see Table 17). However, based on the RS values of the GC peaks and occurrence in the blank, trichlorophenol and fluoranthene are possibly attributable as concentrate production artifacts, as indicated in Table 9.

M2X: XAD-2 extract of RO brine--As explained elsewhere, the M2X concentrate was excluded from Table 9 because of space limitations. The reason M2X was chosen for omission was that it was badly contaminated with XAD-2 resin bleed artifacts. Of 204 non-acidic compounds identified in concentrate M2X, 133 (65 percent) were XAD-2 resin bleed artifacts. In addition, 89 of the 100 largest GC-MS peaks were identified as XAD-2 artifacts. Since the M2X results were omitted from Table 9, they have been included in Appendix B of Volume 2.

Although the XAD-2 artifacts dominated the chromatograms for concentrate M2X, this material was not the predominant substance present. Most of this artifact material was recovered in the aromatic fraction which accounted for only 0.4 percent of the organic material present in the concentrate. In agreement with all of the other XAD-2 produced DW concentrates, M2X consisted of predominantly humic-related material which is not recovered well in the partitioning scheme, and the humic material that is recovered appears predominantly in the acid fraction. For M2X, 88 percent of the material recovered in the fractions was in the acid fraction.

Fluoranthene was the only specific search compound found and may be attributable as an artifact (see discussion of M2C, above). Two isomers of DDE, probably degradation products of DDT, were also identified in M2X. Relatively large components of salicylic acid, dimethylmaleic acid and methylethylmaleic acid were the only other noteworthy compounds found. All four of these compounds were also identified in concentrate M2C. The majority of the non-artifact compounds identified were a large variety of oxygenated compounds (ketones, alcohols, ethers, furans, and furanones).

Comparison of concentrates M2C and M2X--The water from which the Miami concentrates were prepared was a 2280-liter (600-gallon) sample of finished drinking water taken at the Miami waterworks on February 3, 1976. Two features of these two concentrates are in apparent contradiction to the fact that the raw water source was groundwater:

- The finished DW apparently contained higher concentrations of humic-related material than any other DW sampling
- A number of water re-use indicators (salicylic acid, clofibric acid, amobarbital and pentabarbital) were identified.

Humic-related material results from degradation of the lignin substance of plant debris, especially leaves. Thus, it is not surprising to find this material in surface water. Generally, one would expect ground water to be relatively free of these materials. The Miami XAD-2 extracted concentrate, M2X, indicates that the sampled water contained a higher concentration of humic-related material (by factors ranging from 2.0 to 5.3) than the DW from cities with surface water sources expected to contain humic material (Cincinnati, Philadelphia, New Orleans, and Ottumwa). This result is underscored by the unusually high concentrations of humic-related material in the solvent extraction produced concentrate, M2C. No other solvent extract type concentrate approached the levels of humic-related materials that M2C contained. Presumably, this anomaly was caused by an equilibrium displacement effect of the very high levels of this material present in the RO brine during solvent extraction. The relatively high concentration of humic-related material in the sampled water obviously indicates that the DW source groundwater aquifier is not well protected from direct surfacewater intrusion. The detection of the two drugs (pentabarbital and amobarbital) and two drug metabolites (salicylic acid and clofibric acid) support this contention that the groundwater source is not protected from intrusion by contaminated surfacewater and add to it a suggestion that the aquifier is vulnerable to treated or untreated sewage.

New Orleans, Louisiana, January 14, 1976--

N2C: combined solvent extract of RO brine--The dominant species of concentrate N2C was di-n-butylphthalate. This material was probably present as a concentrate production artifact. The specific search compounds and other high interest species detected in concentrate N2C require some comment. The controversial herbicides, 2,4-D and 2,4,5-T, have been found in relatively high concentrations (54 and 11 μg/l, respectively). Only concentrate O2C contained comparable concentrations of these two herbicides (entries 427 and 190, Table 9, for 2,4-D and 2,4,5-T, respectively). A 2,4,5-T isomer was identified at about the same concentration (RS value 3.7), and an even higher concentration (RS value 4.7) of a 2,4-D isomer was also detected. Although not a specific search compound another herbicide, atrazine, has also been detected at relatively high levels (RS value 5.7). Again, O2C was the only other DW concentrate in which atrazine was found. The herbicide, dicamba, was also identified at relatively high concentrations (RS value 4.7). In addition, the pesticides heptachlor and lindane (two isomers) as well as DDE (which may indicate the presence of DDT) were also found by the specific search software. Other highly chlorinated specific search compounds found were pentachlorophenol, 2,4-dichlorophenol, hexachlorobenzene, and hexachlorobutadiene. Phenol, diphenylamine and triphenyl phosphate were the other specific search compounds found. In all, twelve specific search compounds were found in the N2C concentrate (see the discussion, Special Interest Compounds, which appears later in this section). This concentrate contained the third highest number of specific search compounds for DW concentrates. A number of water re-use indicators were identified in the N2C data: clofibric acid, salicylic acid, caffeine, benzoic acid, and BHT.

In the acid fraction, 67 carboxylic acids, of which 44 were aliphatic, were identified. This number of carboxylic acids is second only to concentrate S2C, and the total RS value in N2C for compounds containing the carboxylic acid group is also the second highest among the DW concentrates, 8.5 versus 8.8 for M2C (see the discussion, Occurrence of Molecular Functional Groups, which appears later in this section). The two maleic acids, dimethyl and methyl ethyl, were dominant components in the acid fraction.

Of 73 compounds identified in the aromatic fraction, 30 contained at least one halogen atom and 7 contained bromine. Except for chloroform, all of the possible bromo chloro haloforms were detected. Halogenated hydrocarbons (C_1 to C_4, 17 compounds) were present at higher concentrations than the halogenated aromatics. Most of the other compounds identified were alkyl substituted benzenes, naphthalenes and partially reduced naphthalenes.

Compounds and their relative amounts in the medium polarity and high polarity fractions were not distinctly different from the other two solvent extract concentrates with similar raw water sources (i.e., Philadelphia, P2C and Cincinnati, T1C and T4C). The identified compounds were mostly diester plasticizers, alcohols and alcohol-polyethers, ketones and a few esters and amides. Atrazine, three phosphate esters (triphenyl, tributyl (possibly an artifact) and diethyl pentyl (tentatively identified)), and hexanedinitrile were found in these two fractions.

N2X: XAD-2 resin extract of RO brine--Because of space limitations, the results of two concentrates were omitted from Table 9. Concentrates N2X and M2X were the ones omitted due to heavy contamination from XAD-2 resin bleed materials. For completeness, the identified compounds for these two concentrates are presented in Appendix A of Volume 2. The level of contamination of N2X was somewhat less than that for M2X, but it was so severe that the aromatic fraction required dilution by a factor of 10 to avoid gross saturation of ion current signals. Of 181 non-acidic compounds in concentrate N2X, 90 are XAD-2 resin bleed artifacts, and 71 of 76 compounds identified in the aromatic fraction were artifacts.

The distribution of material among the fractions for concentrate N2X (Table 7) was typical of XAD-2 extracted concentrates and is reflected by the low overall recovery into the fractions (10 percent) and the predominance of the acid fraction in the recovered material (90 percent).

The herbicides, 2,4-D, an isomer of 2,4-D, and dicamba were identified in the acid fraction at comparable concentrations to those found in concentrate N2C. Somewhat surprisingly, 2,4,5-T and an isomer, found in N2C, were not found in N2X. Other acids found in both N2C and N2X include 2 isomers of dichlorobenzoic acid, p-chlorobenzoic acid, methylethylmaleic acid, dimethylmaleic acid and salicylic acid. Three chlorinated acids, dichloroacetic, chlorobutenoic and dichlorobutenoic, were found in N2X but not in N2C, in agreement with the usual trend that relatively stronger acids are more effectively recovered in the XAD-2 extracted concentrate.

The only other noteworthy compounds found in concentrate N2X are α-chloro-acetophenone (phenacyl chloride) which is a lacrimator used in tear gas and chemical mace, bischloroethyl ether, BHT and two isomers of DDE (also identified in N2C). Three specific search compounds were found: phenol, 2,4-D and fluoranthene. The fluoranthene was measured at such a low level (RS value of -0.3) that it would have been attributed to the blank in Table 9 (see entry 933). Phenol was quantified at 11 ng/l in N2X and at 7 ng/l in N2C. Since the quantification is based on the internal standard, phenol-D_5, the difference in these values is probably real and the conclusion is either that the XAD-2 resin contributed phenol as an artifact, or that XAD-2 resin is more effective for the extraction of phenol from RO brine than is solvent extraction. Since phenol was found at comparable levels in the blank XAD-2 concentrate, V1X, which contained very high levels of resin artifacts, the former explanation is probably correct. T1C and T1X are the only concentrate pairs for which phenol was identified in both concentrates and little XAD-2 resin contamination was found. In this case, the solvent extract concentrate, T1C, contained higher levels than the XAD-2 extract concentrate, T1X (see entry 156, Table 9).

Comparison of concentrates N2C and N2X--Concentrates N2C and N2X were prepared from 6620 liters (1750 gallons) of DW sampled at the GSRI laboratories in New Orleans, Louisiana. The amounts of organic material in these two concentrates and the distribution of that material in the partitioned fractions is consistent with other DW concentrate pairs with similar surface water sources. Also consistent with other DW solvent extract and XAD-2 extract concentrate pairs, the N2C and N2X compound identification results have little in common. Omitting compounds attributable as artifacts to XAD-2 resin, only 48 of the 326 different compounds found in these two concentrates were found in both concentrates. Of these 48 compounds, 29 were acids. All of the non-artifact compounds found exclusively in N2X were also polar materials: 23 acids, 14 alcohols, 18 ketones, 3 highly polar neutrals (for example, N-hydroxyphthalamide), and 22 medium polarity neutrals (for example, esters, ethers, and amides). In contrast, many highly apolar neutrals were identified in concentrate N2C (for example, 73 compounds in the aromatic fraction).

The levels of herbicides found in these two concentrates is consistent with the agricultural drainage into the Mississippi River. While there are several chemical industry sources of organic pollution of this source water, indicative compounds are relatively few compared to those for DW concentrates from Cincinnati and Philadelphia.

Philadelphia, Pennsylvania, February 10, 1976--

P2C: solvent extract of RO brine--With respect to organic material recoverable by solvent extraction of RO brine, the DW sampled at Philadelphia was about average, with the concentrate reflecting a concentration of 177 ng per liter of sampled DW (Table 7). The organic material in concentrate P2C was, however, somewhat different from the other concentrates in the amount which was recoverable as the high polarity fraction. This fraction represented 32 percent of that present in the P2C concentrate. Values for other solvent extract type concentrates ranged from 10 percent for T4C to 20 percent for S2C and averaged 15.3 percent. Thus, the P2C concentrate contained a significantly higher relative amount of these high polarity materials than comparable concentrates. The relative amounts of the concentrate recovered in the other fractions (Table 7) were not significantly different from those for other solvent extract concentrates.

The types of molecules found in the high polarity fraction are not significantly different from those found for comparable concentrates. The percentages of the identified compounds in which the usual functional groups were found are as follows: 38 percent contained the hydroxyl group, 29 percent contained the keto group, 23 percent contained the ether group, 5 percent contained the aldehyde group, and 15 percent contained a ring hetero atom. Only five diester plasticizers were identified. Dibutyl phthalate was found at very high concentration and is judged to be an artifact introduced during concentrate preparation at some point following RO processing. Nearly identical contamination was found for concentrates M2C and N2C.

Four species of isopropylidine derivatives of sugars (entries 12, 13, 238, and 502, Table 9) were identified at high levels (up to the RS value 6.8) in the high polarity fraction. These compounds occurred in two other cases (the DW concentrate, O2C, and the AWT concentrate, R2C, Table 10). However, detection of one of these (entry 12, Table 9) in the extraction solvent blank (T1C) makes interpretation difficult.

Another distinguishing characteristic of the high polarity fraction of P2C is that it contained higher levels of poly glycol ethers than any other DW concentrate. A measure of the amounts of these materials present can be taken from the RS values for the entries for tripropylene glycol methyl ether isomers in Table 9 (entries 101, 102, 203, 204, 243, and 581). This class of compound is usually present as oligomers of poly ethylene and poly propylene glycol with a range of ethers as the terminal group. Thus, the set of tripropylene glycol methyl ether isomers is only a minor component. Usually, these oligomeric species could not be identified specifically for entry into the database as a molecular structure, and, therefore, few appear in Table 9. Thus, occurrence in P2C of these species at the highest levels seen in DW concentrates is based on the GC-MS chromatograms of the high polarity fraction rather than the results shown in Table 9. Certainly, the relatively higher levels of these materials in P2C must partially account for the higher recovery into this fraction for concentrate P2C.

The acid fraction had the following distinguishing features:

- Benzoic acid, clofibric acid and salicylic acid (water re-use indicators) were among the components identified at higher concentrations (RS values of 5.8, 5.8, and 4.8, respectively)
- Dimethylmaleic acid and methylethylmaleic acid were found at relatively high concentrations (RS values of 5.8 and 4.8, respectively)
- Five multichlorinated, low carbon number acids were identified (dichloroacetic, dichloroacrylic, trichloroacrylic, dichlorobutenoic and pentachloropentadienoic which is a degradation product of hexachlorocyclopentadiene)
- p-Chlorophenol, 2,4-dichlorophenol, 3,5-dichlorophenol and 2,4,6-trichloro phenol were identified
- Fatty acids above C_{12} were absent. The carboxylic acids were about evenly distributed both in numbers and total amounts between aromatic and nonaromatic species.

The aromatic fraction contained a large number of halogenated materials (24 compounds, 34 percent of the total), most of which were non-aromatic. Some of the noteworthy identifications are:

- Bromocyclohexane, iodocyclohexane, 1-iodopentane and 2-iodopentane
- Trichloroaniline and two isomers of dichloroaniline
- Ortho, meta and paradichlorobenzene and hexachlorobenzene
- Styrene, 2-methylstyrene, and 2-chloronaphthalene.

The above compounds strongly indicate contamination from chemical industry sources. However, only one of the above compounds had an RS value greater than 1.8 (iodocyclohexane at 2.8), so the level of contamination may not be objectionable.

The medium polarity fraction also contained some chemical industry pollution indicators: phenylacetonitrile, benzonitrile, ethyl and dimethyl pyridine, isophorone, DMF, diphenylamine, and four aldehydes. As usual, the balance of the compounds were ketones, alcohols, esters and plasticizers.

P2X: XAD-2 extract of RO brine--Among the XAD-2 produced concentrates, P2X had next to the lowest overall recovery of material into the fractions at 7.7 percent. This value would have been even lower had it not been for a relatively higher amount of material in the high polarity fraction. This result mirrors that for the solvent extract concentrate, P2C, which had the highest relative recovery for this fraction of all the DW solvent extract concentrates (Table 7).

Concentrate P2X was substantially contaminated with material attributable as XAD-2 resin bleed but less contaminated than the two concentrates, M2X and N2X, which were omitted from the listing of Table 9 on that basis. Of the XAD-2 produced concentrates listed in Table 9, concentrate P2X had the most compounds (86) classified as XAD-2 resin bleed. For comparison, the numbers of identifications classified as artifacts for concentrates O2X, T2X, S2X, T1X, and T1Y were 60, 56, 12, 2, and 22, respectively. Thus, the P2X results in Table 9 give the most representative characterization of what chemical species constitute XAD-2 resin bleed material. See also Appendix A of Volume 2 and discussion of the Jefferson Parrish results in Volume 3 for similar information.

Four specific search compounds (Table 4) were identified in P2X. Styrene is without doubt an XAD-2 resin artifact even though it was also found in concentrate P2C. Fluoranthene, which was not found in P2C, should also be classified as a resin bleed artifact since it was also detected in the blank concentrate, V1X, which was very heavily contaminated with XAD-2 resin bleed artifacts. Trichlorophenol was identified in P2C at a concentration about 30 times higher than in P2X while pentachlorophenol (found at 0.6 ng/l in P2X) was not found in P2C. It is somewhat surprising that extraction efficiencies would favor recovery of trichlorophenol but not pentachlorophenol in P2C, and the possibility remains that the pentachlorophenol in P2X is actually an artifact.

In the acid fraction of P2X, the strong acid herbicide, dicamba, was identified. This compound was not identified in concentrate P2C. Some of the stronger or more polar acids identified in P2C were also identified in P2X: trichloroacrylic, dichloroacetic, dichlorocrotonic, phthalic, azelaic, suberic, sebacic, salicylic, o-anisic, and anisic. The number of non-aromatic acids identified exceeded the aromatic acids by about 3 to 2.

Essentially all of the 90 compounds identified in the aromatic fraction can be classified as definite or probable XAD-2 resin bleed artifacts. For the medium polarity fraction, 17 of the 42 identified compounds (40 percent) also must be classified as XAD-2 resin artifacts. In this case, 7 of the artifacts are ethyl esters of fatty acids and, thus, do not originate from the resin but from esterification of fatty acids in the sample with the ethyl alcohol solvent. Bischloroethyl ether is the only noteworthy compound detected in this fraction.

The XAD-2 resin artifact interference extends even to the high polarity fraction with 10 of the 37 compounds (27 percent) attributable as resin bleed. Most of these compounds are arene substituted acetophenones with ethyl stryene and proprophenone also present. Isophorone is the only noteworthy compound found in this fraction. The balance of the non-artifact compounds are alcohols (7 compounds), ketones (8 compounds), and poly glycol ethers (9 compounds). A number of poly glycol oligomers were also identified generically, but these were not added to the database since not enough was known about their molecular structures.

Comparison of concentrates P2C and P2X--The concentrates P2C and P2X were prepared from 5810 liters of DW sampled at Philadelphia's Torresdale Waterworks on February 10, 1976. As for other solvent extract and XAD-2 extract pairs of DW concentrates, the compound identification results for P2C and P2X have little in common. Omitting the compounds attributable to XAD-2 resin bleed in the P2X concentrate, only 15 percent (56 ot 370) of the compounds identified in these two concentrates were found in both concentrates. The correspondence between these two concentrates would be somewhat better if the large amount of XAD-2 resin bleed artifacts did not present such a high level of interference. Consistent with the other corresponding DW concentrate pairs, most of the compounds found exclusively or at significantly higher concentrations in the XAD-2 produced concentrate (P2X) are relatively stronger acids or more polar materials.

The total amount of organic material in the P2C and P2X concentrates (equivalent to 1,180 µg per liter of original water) was about midway in the range for the samplings shown in Table 7 (136 µg/l for Seattle to 2630 µg/l for Miami). The distribution of the concentrate material among the fractions was also fairly typical for these two concentrates. Concentrate P2X had the lowest percentage of material recovered in the acid fraction for all DW XAD-2 extracted concentrates suggesting that humic-related material may have been present in this concentrate at slightly higher levels than in other XAD-2 extracted concentrates. In addition, concentrate P2C yielded the highest recovery observed in the high polarity fraction while the P2X recovery for this fraction was the second highest. This result was apparently due to higher relative amounts of poly glycol oligomers and non-aromatic alcohols and ketones.

In summary, the compound identification results for concentrate P2C indicate the presence of chemical industry effluents in the source water although the levels of these materials are not higher than those for comparable samplings (for example, Cincinnati and New Orleans).

Ottumwa, Iowa, September 10, 1976--

O2C: combined solvent extract of RO brine--The concentration of organic material which the O2C concentrate represented in the sampled DW was 139 μg/l. This concentration is somewhat lower than the average (163 μg/l) for the other DW concentrates with a reasonably similar surface water source (143, 115, 217 and 177 μg/l for T1C, T4C, N2C, and P2C, respectively, Table 7). The overall recovery of concentrate O2C into the analyzed fractions was 57 percent, the second highest recovery obtained for solvent extract concentrates. However, this recovery was not significantly different from the other solvent extract concentrates (except the highest, 65 percent, for P2C; see Table 9).

The identified compounds with the largest GC-MS peaks in the acid fraction were the ubiquitous dimethyl- and methylethylmaleic acids. However, these two substances may have been present in the concentrate predominantly as the anhydrides, with the methyl ethyl species being the largest GC-MS peak found on GC-MS analysis of the unpartitioned concentrate. Whether the free acids of these two anhydrides were also present in the unpartitioned concentrate is not known since the gas chromatographic or mass spectrometric characteristics for the free acids were not investigated. However, the anhydrides were not found in any of the analyzed fractions, and the fractionation pH extremes would be expected (based on the reported data for maleic anhydride) to convert all of the anhydride to the free acid. The nitrogen analogues to these two maleic anhydrides were also detected in the unpartitioned concentrate. Presumably, the maleimides would hydrolize to the corresponding acid-amide species during partitioning. However, no specific attempt was made to find these materials in the GC-MS data. These four species (two anhydrides and two imides) were added to the computer database even though they were not found in the acid fraction since they were found in the original concentrate.

Concentrate O2C also contained the highest level of 2,4,5-T (15 ng/l) seen for the DW solvent extract concentrates. A smaller quantity of 2,4-D (4 ng/l) was also detected. For comparison, the relative levels of 2,4,5-T and 2,4-D were reversed in T4C at 5 and 44 ng/l, respectively, and in N2C at 11 and 54 ng/l, respectively, while in T1C (the only other solvent extract in which the two phenoxy herbicides were found) the levels were in the same order at 5 and 2 ng/l for 2,4,5-T and 2,4-D, respectively. Another herbicide identified in O2C was atrazine with an RS value of 2.9 (entry 91, Table 9). The only other concentrate in which this compound was found was the New Orleans concentrate, N2C, with an RS value of 5.7.

Pentachlorophenol, p-chlorophenol and phenol were found in the acid fraction with the RS values 3.9, 1.9 and 0.9, respectively. The detection of phenol here is low enough to be attributable to the blank. A number of alkylbenzoic acids were found (2-methyl, 5 isomers of dimethyl and 4 isomers of trimethyl). Two isomers of clofibric acid and salicylic acid were detected at levels comparable to those for other concentrates. The ratio of non-aromatic species to aromatic species in the acid fraction was about 4 to 3.

The aromatic fraction contained few of the chlorinated aliphatic and aromatic hydrocarbon and other species which have been taken to indicate the presence of contamination from chemical industry sources. The five halogenated species found were two isomers of trichloropropene, a dichloropentane isomer, iodocyclohexane and o-dichlorobenzene. The other 42 compounds identified were alkylated and/or alkenylated benzenes (28 species), naphthalenes (5 species), partially reduced naphthalenes, indenes and azulenes (6 species), biphenyls (2 isomers) and stilbene. This set of compounds is similar in both type and relative concentrations to a subset of compounds that are usually ascribed to XAD-2 resin bleed artifacts, with the most abundant species being the diethylbenzenes, ethyl styrenes and naphthalene. However, concentrate production did not involve contact with XAD-2 resin. Furthermore, the many biphenyl, and bisphenyl C_1 and C_2 species always observed in the XAD-2 artifact profile were not detected. If these materials were not artifacts, then a reasonable explanation might be contamination of the source water by diesel fuel and/or gasoline (explaining the presence of some of the substituted benzenes and partially reduced naphthalenes) as well as contamination from a polystyrene/divinylbenzene source (explaining the relatively high concentrations of ethyl styrenes and related species).

The high polarity fractions contained an isopropylidine derivative of a sugar (furanose) which gave the largest GC-MS peak. Four such components were also identified as major compounds in the P2C concentrate but not in any other concentrates. Isophorone, atrazine, triethylphosphate and diethyl sulfite, and 7 aldehydes were detected in this fraction also. Comparatively, plasticizers and poly glycols were not major constituents of this fraction. Most of the identified compounds contained the hydroxyl (18 species) and/or the keto (28 species) functional group.

The medium polarity fraction contained diethylformamide, 2,4,6-collidine and six aldehydes. There were also six ethyl esters of fatty acids, compounds which are usually associated with XAD-2 resin produced concentrates.

O2X: XAD-2 resin extract of RO brine--Although concentrate O2X resulted in the lowest overall recovery of material into the analyzed fractions (6.5 percent, Table 7), it should not be considered atypical. The low overall recovery into fractions (6.7 percent), the predominance of acid fraction among the others (90 percent of the recovered material) and the pronounced, late eluting profile of unresolved material in the GC-MS chromatogram of the acid fraction on the SP2100 column were typical among the XAD-2 prepared DW concentrates.

As with all XAD-2 resin produced concentrates (except T1X, T1Y, and S2X), O2X contained a significant amount of artifact material attributable to the XAD-2 resin. These artifacts constituted a major portion of the material in the concentrate identifiable by GC-MS analysis. Of the 231 compounds listed in Table 7, 60 were attributable to XAD-2 resin bleed and 29 to other concentrate production method sources. Only 5 of the 61 compounds identified in the aromatic fraction were not probable XAD-2 resin artifacts. In this instance, however, the relative amounts of lower molecular weight material (substituted benzenes) and higher molecular weight material (bisphenyl species) was the opposite of that observed for the M2X, N2X, and P2X concentrates. In the present case (O2X), the bisphenyl species were the predominant ones. Also in contrast to the results for M2X, N2X, and P2X, naphthalene (as an artifact) was observed at a concentration about 5 to 8 times that of the predominant bisphenyl species and about 15 to 50 times those for the substituted benzene species.

In the acid fraction, two specific search compounds were found: phenol and 2,4-D. Since phenol was found at about 10-fold higher concentration in O2X compared to O2C, it should probably be considered present in O2X as an artifact. Results from other XAD-2 prepared concentrates have suggested phenols as a possible resin bleed artifact also. The two maleic acids (dimethyl and methylethyl) which were the most concentrated components of the O2C acid fraction were among the largest GC peaks of O2X also. Other compounds of interest include salicylic acid and ethosuximide as water re-use indicators. The strong acids usually more prominant in XAD-2 prepared concentrates included four chlorinated acids (C_2 through C_4) and six alkanedioic acids (C_2, C_4, C_8, C_9, C_{10}, and C_{11}).

The high polarity fraction contained nicotine, isophorone and the usual array of alcohols and ketones. While the usual diester plasticizers were present, they were at lower levels than often encountered. The medium polarity fraction contained some noteworthy nitrogen containing compounds: nicotine, 2,6-lutidine, 5 quinoline/isoquinoline species, and N,N-dimethylbenzylamine.

Comparison of concentrates O2C and O2X--The water from which the O2C and O2X concentrates were prepared was a 5450-liter (1440-gallon) sample of finished DW taken on September 10, 1976, at the Ottumwa, Iowa, waterworks. The source water was the Des Moines River for which the city of Des Moines, about 90 to 120 miles upriver, is presumed to be the only significant non-agricultural source of pollution. The results of analysis of the O2C and O2X were consistent with reasonable expectations of the source water:

- Herbicides 2,4-D, 2,4,5-T, and atrazine were found at levels comparable to the highest observed in other DW concentrates from agricultural drainage surface water (New Orleans, Cincinnati, and Philadelphia).

- In comparison with other DW concentrates from surface water sources, few compounds were found indicating significant pollution from chemical industry sources
- Most of the organic material present in the XAD-2 produced concentrate, 02X, was humic-related
- Some of the standard water reuse indicators (salicylic acid, clofibric acid, ethosuximide and nicotine) were present at relatively moderate levels while other reuse indicators (benzoic acid, phthalates and poly glycol ethers) were found at levels lower than those found for other concentrates with surface water sources.

A particularly curious aspect of the 02C and 02X compound identification results was that the set of compounds found in the aromatic fractions for both concentrates constituted a reasonable representation of the usual spectrum of XAD-2 resin artifact compounds) however, the lower molecular weight substances (substituted benzenes and partially reduced naphthalenes) were predominantly in the 02C concentrate while the higher molecular weight materials (bisphenyl compounds) were predominantly in the 02X concentrate. The nature of this anomaly can easily be visualized by scanning the entries for 02C and 02X in Table 7 and comparing occurrence and RS values of compounds designated as XAD-2 artifacts for these two concentrates with other solvent extract and XAD-2 extract pairs (T4C, T4X; P2C, P2X; and S2C, S2X). One possible explanation is that the substituted styrene species might be from the effluent of a polystyrene plant upriver and the other species were due to gasoline or fuel oil contamination. However, another curious aspect is that 02C contained 6 ethyl ester species which are usually ascribed as artifacts due to esterification from the ethanol solvent of XAD-2 type concentrates. Ethyl esters were rarely found in solvent extract concentrates. Without further information regarding the source water, these observations will have to remain engmatic.

Comparison of the identified compounds for these two concentrates indicates the usually observed mutual exclusivity for solvent extract/XAD-2 resin concentrate pairs. Enumeration of the results shown in Table 7 for 02C and 02X shows that only 43 of 309 compounds (14 percent) were detected in both concentrates. The compound occurrence data is generally consistent with the usual characterization that the most polar compounds are recovered more efficiently by XAD-2 extraction of the RO brine while the least polar compounds are nearly exclusively recovered by solvent extraction of the RO brine.

Seattle, Washington, November 5, 1976--

S2C: combined solvent extract of RO brine--Concentrate S2C represented the lowest concentration of organic material in the corresponding source water (37 μg/1, Table 7) of all the non-blank concentrates that were analyzed. However, since a very large volume of DW (11,750 liters) was sampled to produce this concentrate, the 10 percent of the concentrate that was used for analysis, at 44 mg of material, exceeded by a factor of two that for concentrate T1C, at 21 mg of material. The amount of material in the analyzed aliquot is equal to 0.1 times the product of the concentration and the volume shown in Table 7. The average for the 7 solvent extract concentrates of Table 7 was 81 mg of organic material in the analyzed aliquot. For concentrate S2C, the distribution of organic material among the fractions and the overall recovery (53 percent) were consistent with the other solvent extract type concentrates of Table 7. In striking contrast, however, is the number of identified compounds shown for S2C, 361 after correction for the blank, compared to an average of 206 for the other solvent extract concentrates of Table 7. Comparing the numbers of compounds identified in the individual fractions of S2C (90, 81, 85 and 160 for acid, aromatic, medium polarity and high polarity, respectively) with the averages for the other six solvent extract type concentrates (73, 49, 45 and 71, respectively, as above), it is clear that, while there was somewhat more identifiable material in the acid and aromatic fractions of S2C, the medium and high polarity fractions contained distinctly more identifiable material than the other solvent extract type concentrates. Comparing the numbers of confirmed versus tentative identifications for the solvent extract concentrates in Table 7, it is obvious that a smaller portion of the identified compounds have confirmed status in S2C. The confirmed:tentative ratio for S2C is 1:2.24 while the average of the other 6 solvent extract concentrates is 1:1.4. The explanation for this apparent anomaly is that only a few of the abnormally high number of identifications in the medium and high polarity fractions of S2C, cited above, have been confirmed. For example, of the 160 compounds identified in the high polarity fraction, only 7 (4 percent) had confirmed identifications. For the medium polarity fraction, only 28 percent of the identifications were confirmed. In contrast, 50 and 41 percent of the compounds identified in the acid and aromatic fractions, respectively, were confirmed. Alcohols and ketones make up the bulk of these excess compounds, and this result can be easily visualized by scanning the listings under the S2C heading in Table 9 and noting the types of compounds that were either found exclusively in S2C or only in S2C and one or two other concentrates. Of 160 compounds found in the high polarity fraction, there were 108 alcohols and/or ketones. These 108 compounds consisted of 26 saturated alcohols, 10 unsaturated alcohols, 9 alcohols with other functional groups, 20 saturated ketones, 23 unsaturated ketones, 12 ketones with other functional groups and 8 compounds with the furan-2-one moiety. The source of this plethora of compounds may be related to the conifer forested watershed which is the source of the raw water since 5 compounds related to oxygenated diterpenes were identified: camphor, pinacol, fenchone, citronellol and farnesol. The above noted alcohols and ketones, in the many unsaturated and alicyclic variations identified, are definitely suggestive of what one might expect for breakdown products of diterpene-related compounds. The mass spectra for these compounds almost never contain the molecular ion as a significant fraction of the ionization. As a result, many identifications of these alcohol/ketone compounds have been made with a significantly lower level of confidence than was possible for other types of functional groups. Since most of these compounds were considered to be relatively innocuous and/or possibly isolated instances of occurrence, identification confirmation was not pursued.

The most distinguishing characteristic of the acid fraction was the relatively higher numbers and concentrations of fatty acids: 38 non-aromatic carboxylic acids with many isomeric forms were identified. Alkyl benzoic acids were also in relatively high abundance with 13 species identified: benzoic; monomethyl, all 3 isomers; dimethyl, all 6 isomers; trimethyl, 2 isomers; and one isopropyl isomer. As usual, methylethyl- and dimethylmaleic acids were among the species present at highest concentration. The chlorinated materials identified were the search compounds 2,4,6-trichlorophenol and pentachlorophenol (1.6 and 0.9 µg/l, respectively) and some chlorinated carboxylics (RS values are in parentheses): dichloroacetic (3.2), trichloroacetic (4.2), dichloropropanoic (3.2), 2-chlorobenzoic (3.2), 2,4-dichlorobenzoic (2.2), 3,4-dichlorobenzoic (2.2), and 2,5-dichloro-4-methylbenzoic (2.2) acids; the herbicides amiben (3.2; 3-amino-2,5-dichlorobenzoic acid) and dicamba (2.2; 2-methoxy-3,6-dichlorobenzoic acid), and pentachloropentadienoic acid (3.2; oxidative degradation product of hexachlorocyclopentadiene). As for the other concentrates, methylethylmaleic acid and dimethylmaleic acid were predominant components, with the former appearing as one of the largest GC peaks in the acid fraction. Two resin acids, dehydroabietic acid and deoxypodocarpic acid, were also identified.

In the aromatic fraction, a greater than normal portion of the compounds contained chlorine (28 of 80 compounds, 35 percent), but only two compounds contained bromine or iodine (dibromochloromethane and iodocyclohexane). Half of the identified compounds contained a discrete benzene nucleus. The specific search compounds found in the aromatic fraction were the following (concentrations, ng/l, are shown in parentheses): lindane (15.), o-chlorotoluene (0.07), p-dichlorobenzene (1.7), 1,2,4-trichlorobenzene (0.04), PCB (Cl_5) (not quantified), styrene (0.09), o-methylstyrene (0.1) and diphenyl amine (0.2). Other noteworthy compounds found were dichloroaniline, trichloroaniline and dichloronitrobenzene. While the above compounds seem to suggest contamination from industrial sources, the concentrations found were quite low with the following numbers of compounds having the indicated RS values: one compound at 3.2, 7 at 2.2, 16 at 1.2, 23 at 0.2, and 33 at -0.8.

As noted above for the S2C concentrate, the medium polarity fraction contained more identifiable compounds than usual. Most of these materials were alcohols and ketones with the alcohols more prevalent in the high polarity fraction and the ketones more prevalent in the medium polarity fraction. Of the 85 compounds identified in the medium polarity fraction, 32 contained a ketone group and 15 contained an alcohol group. Three of the four largest GC-MS peaks in the fraction were chlorinated alcohols and ketones. The only specific search compound identified in the medium polarity fraction was 2-chloroaniline at 3 ng/l. Other noteworthy compounds included (RS values are in parentheses): methyl isocyanate (2.2), DMF (1.2), phenylacetonitrile (1.2), and dimethyl sulfone (2.2).

The analysis results for concentrate S2C can be summarized as follows:

- The RS values of the identified compounds were uniformly lower than those for other concentrates. This result was principally attributable to the very large volume of the sampling.

- An unusually large number of ketone and alcohol compounds were identified and these two classes of compounds account for the comparatively larger number of compounds identified in the concentrate. Most of these ketone and alcohol compounds were in the C_6 to C_{10} range and may be related to breakdown products of oxygenated diterpenes.
- Considering the source of the water, many of the non-aromatic chlorinated compounds probably originated from chlorination at the treatment plant rather than contamination from anthropogenic sources.
- Some of the ubiquitous water re-use indicators (for example, clofibric acid and salicylic acid) were not detected in concentrate S2C, consistent with expectations based on the source of this water. Other water re-use indicators such as plasticizers and poly glycols were found at lower levels and in few cases.

S2X: XAD-2 extract of RO brine--The usual late eluting profile of humic-related material in the acid fraction GC-MS chromatogram on the SP2100 column was distinctly less pronounced for the S2X concentrate than for most of the other XAD-extracted concentrates. However, the overall recovery of 12 percent of the concentrate material into the fractions was comparable to, but at the upper range of, the other 6 XAD-2 concentrates. Thus, it appears that either the nature of the humic-related material or the relatively lower total amount that was present in the partitioned aliquot (about one fourth the average for T4X, M2X, N2X, P2X, and O2X) resulted in less interference in the acid fraction than usual. Another characteristic of concentrate S2X that enhanced the quality of the GC-MS data was that few XAD-2 resin bleed artifacts were present. Only 12 of the 171 compounds detected for S2X are indicated in Table 9 as possible or probable XAD-2 resin bleed artifacts. Only one concentrate showed fewer XAD-2 artifacts (T1X, produced by the HERL laboratory staff), and the others were at least an order of magnitude worse in this respect.

The most concentrated components of the acid fraction were a series of dihydroxy-alkyl-benzoic acids which probably originate from degration of lignin in the extensive forested watershed of the source water. Some analogues with one or more methoxy groups substituted for hydroxyl groups were probably from the same source. Salicylic acid and ethosuximide were the only water re-use indicators identified in the acid fraction. The chlorinated herbicides dicamba and dalapon, also identified in S2C, were the only herbicides detected. Consistent with essentially all the other concentrates, methylethylmaleic acid was among the most abundant materials identified, and dimethylmaleic acid was also identified but at a substantially lower concentration. In proportion to the total number of compounds identified in the acid fraction, a relatively large number of chloro non-aromatic carboxylic acids were identified: chloroacetic, dichloroacetic, 2-chloropropenoic, trichloropropenoic, 2,2-dichloropropanoic (dalapon), 2,2-dichlorobutanoic and 4,4-dichlorobutenoic acids. p-Nitrobenzoic, phthalic, terephthalic and 2-chlorobenzoic acids (relatively stronger and more polar species) were found at moderate levels while the less polar fatty acids (predominant in S2C) were only minor components. A relatively large amount of benzoic acid was probably at least partially attributable as an XAD-2 resin bleed artifact. Three isomers of methylbenzoic acid and three isomers of dimethylbenzoic acid, detected at lower concentrations than for S2C, may not be attributable as XAD-2 artifacts.

All seven of the specific search compounds detected were found in the aromatic fraction (concentrations, ng/1, are shown in parentheses): p-dichlorobenzene (0.7), lindane (0.3), pentachlorobiphenyl and other PCBs (less than 0.1), o-chlorotoluene (0.06), trichlorobenzene (0.02), diphenylamine (0.02), and fluoranthene (less than 0.01, possibly an XAD-2 resin bleed artifact). All of these specific search compounds were also found in concentrate S2C. Only about three of the 44 compounds found in this fraction were attributable as XAD-2 resin bleed artifacts. Similarly to S2C, nearly half (19) of the compounds contained halogen, and 13 of these were nonaromatic. Typical compounds were three isomers of trichloropropene, three isomers of dichloroisopentane, bromocyclohexane and chlorocyclohexane. Most of these compounds, and other similar ones, were also identified in concentrate S2C at about the same concentrations. Since these compounds should have been nearly completely recovered from the RO brine by solvent extraction (and, therefore, in concentrate S2C), they should have been absent or present at far lower concentrations in concentrate S2X. Since this was not the case, the possibility remains that they may be artifacts. In support of the postulated lignin breakdown products found in the acid fraction, three substituted naphthalene compounds which could have originated from resin acid decomposition were identified in the aromatic fraction. Two other compounds of interest are 2,4,6-trichloroaniline and dichlorocyclooctadiene. The latter compound may be a dimerization product of chloroprene.

The medium and high polarity fractions present no anomalies or other unexpected results. The numbers of alcohols and ketones identified are essentially normal in contrast to the plethora of these species in S2C, but this is the expected result based on the solvent extractability of these materials. Plasticizers and poly glycols were fewer in number and lower in concentration compared to the low levels found in S2C, as would be expected. There were more XAD-2 resin bleed artifacts identified in the medium and high polarity fractions than in the acid and aromatic fractions. A total of 7 and 6 XAD-2 resin bleed artifacts were identified for the medium and high polarity fractions, respectively, in addition to 4 fatty acid ethyl esters arising from the ethanol solvent. Nicotine, isophorone, 1-methylisoquinoline and diethylformamide were the only compounds of potential interest which were identified.

Comparison of concentrates S2C and S2X—The S2C and S2X concentrates were prepared from 11,750 liters (3100 gallons) of finished DW sampled on November 5, 1976, at the distribution system at 2700 Airport Way in metropolitan Seattle. The raw water source for the sampled DW was reported to be the Cedar River.

There was the usual high degree of mutual exclusivity in the identification results for S2C and S2X which was consistent with that observed for other solvent extract/XAD-2 extract pairs of DW concentrates. In this case, only 61 of the 441 compounds identified in these two concentrates (14 percent) were identified in both concentrates. Corresponding values for the other concentrate pairs ranged from 12 to 20 percent.

The distribution of recoveries into the fractions for these two concentrates were not significantly different from those of the other concentrate pairs. The values for S2X indicate the typical poor overall recoveries due to the presence of humic-related material. However, in this case, the presence of the humic-related material did not result in the usual quantities of interfering material in the acid fraction. In addition, the near absence of XAD-2 resin bleed artifacts in S2X also enhanced the ability to detect sample constituents at low levels. The result of these two factors was that a relatively higher number of the S2X identifications were also found in S2C: 61 of 140 compounds (44 percent). The corresponding values for the other 6 concentrate pairs ranged from 24 percent to 37 percent and averaged 33 percent.

No water re-use indicators were identified in concentrate S2C, as expected, based on the source of the water. However, three high polarity re-use indicators were identified in concentrate S2X (RS values are in parentheses): salicylic acid (3.2), ethosuximide (3.2), and nicotine (0.2). With one exception, ethosuximide has been identified only in XAD-2 produced concentrates. Similarly, in 4 of 6 identification instances, nicotine was found only in the XAD-2 produced concentrate, and in the one case of identification in both the solvent extract and XAD-2 extract concentrates (T1C and T1X), the XAD-2 produced concentrate contained a significantly higher level. Salicylic acid was found in all the XAD-2 produced concentrates and all solvent extract concentrates except for S2C. There is no readily apparent explanation for this anomaly other than the S2X detection was as an artifact or detection in S2C was obscured by interfering materials.

In summary, the results for these two concentrates suggest the following characteristics for the original water:

- The low levels and numbers of drugs, drug metabolites, plasticizers and poly glycol species indicate the presence of a small but distinct component of re-use water.
- Chlorination has apparently given rise to a substantial number of non-aromatic chlorine containing species of relatively low molecular weight. In this context, the lack of companion brominated species probably derives from the assumed extremely low level of bromide ion in the source water.
- Most of the organic material in the water can be attributed to non-anthropogenic sources in the forested watershed as indicated by the variety of oxygenated diterpene-related and resin-related species detected.

The very large number of alcohols and ketones found were postulated to be breakdown products of oxygenated diterpene-related materials.

- There was only a slight indication of the presence of industrial chemicals although there was evidence of the use of pesticides and herbicides in the watershed (dicamba, dalapon, amiben and lindane).

Comparison and Discussion of DW Concentrate Analysis Results

The Degree to Which the GC-MS Analysis Results Characterize the Organic Concentrates—

A central conclusion of this work is that most of the organic material present in the concentrate was not accessible to the type of detailed molecular characterization provided by GC-MS analysis. The recovery results for partitioning of the concentrates prior to GC-MS analysis (Table 7) clearly show that most of the organic material present in the concentrate was not recovered into the four fractions on which essentially all of the compound identification results were based. The average recoveries were 52 percent and 10 percent for the 7 solvent extract and 7 XAD-2 extract concentrates, respectively. Combining recoveries for each pair of solvent extract and XAD-2 extract concentrates yields composited recoveries for each sampling which range from 14 percent (Ottumwa, Iowa) to 25 percent (Cincinnati, Ohio, January 14, 1980) and average 20 percent. Evidence is presented in the section "Results and Discussion, Overview", which support the contention that most of the approximately 80 percent non-recovered material was humic-related substance. Certainly, other classes of compounds, such as quaternary ammonium ions, mono- and diphosphoric esters, organosulfonic acids, polyhydroxy species (for example, glycerol and manitol) and other highly polar and/or ionizable species (for example, citric acid and ethanolamine) represent a portion of the 80 percent which was not recoverable through the partitioning scheme, but the limited evidence, cited above, indicates that humic-related materials are the major fraction of these non-recoverable substances. Thus, one must remain cognizant that the compound identification results presented here represent less than 20 percent (as the average) of the organic material that was present in the originally sampled DW. Actually, the fraction of organic material which the identified compounds represent may be significantly less than 20 percent since (1) there is good reason to believe that the RO process failed to retain many GC-MS analyzable species, and (2) it is clear that a major portion of the recovered material in the acid fraction was not sufficiently volatile for gas chromatographic analysis. Failure of the RO process to recover many GC-MS analyzable organic species was addressed in the discussion section in which the T1Y results were compared with the combined results of T1C and T1X. Based on that comparison, and assuming that the lost organic material escapes into the RO permeate rather than being lost to absorption on the membrane surfaces, a more effective method for preparation of representative organic concentrates would be RO concentration followed by direct XAD-2 adsorption of the RO permeate water at both acidic and basic pH.

Compounds Identified in Most of the Concentrates--

Inspection of Table 9 conveniently visualizes the frequency with which compounds were found in the DW concentrates. Not surprisingly, compounds which were identified in most of the concentrates were usually found, in at least one of the detection instances, with RS values at the upper end of the range. Thus, these compounds appear toward the beginning of Table 9. Depending on the molecular properties, a compound might be exclusively recovered into either the solvent extract concentrate or the XAD-2 extract concentrate or both. This factor must be kept in mind when scanning Table 9 for frequently identified species.

Some of the frequently detected compounds in Table 9 are itemized below. Numbers in parentheses following compound names designate the entry sequence number in Table 9.

- Ethylmethylmaleic acid (7) was found at or near the highest levels observed for identified components in the acid fractions of every DW concentrate except the Poplarville, Mississippi, blank. The related compound, dimethylmaleic (14), was also present at about one-third to one-tenth the level of the ethylmethyl species. That these materials were not artifacts is confirmed by their absence from all of the analyzed blank concentrates (V1C, V1X, X1C, X1X, and T2B) and their presence in non-RO produced small-volume samples of the Cincinnati, January 14, 1980, set (reported in Volume 3). These two acids are probably related to environmental degradation of polyester (alkyd) resins widely used in paints and other polymer applications. The remarkable ubiquity of their detection and both the uniformity of the concentrations observed and the relative amounts of the two species in each concentrate suggest that they may be highly refractory toward biodegradation in surface waters.
- Fatty acids were always present as a fairly standard set of species but often at different levels from one concentrate to another. Since fatty acids were also often detected in concentrate blanks and partitioning blanks, many of the detection instances of Table 9 for these species (especially ones between C_{12} and C_{18}) have been attributed to the blank. It is reasonable that in most cases some portion of the fatty acid actually came from the sampled water. The fatty acids detected with the highest frequencies were: stearic, C_{18} (52); oleic, C_{18}-ene (88); palmitic, C_{16} (4), myristic, C_{14} (18); lauric, C_{12} (86); capric, C_{10} (82); pelargonic, C_9 (51); caprylic, C_8 (48); 2-ethylhexanoic (71); heptanoic (158); caproic, C_6 (155); 2,3-dimethylbutyric (517); valeric, C_5 (95); isovaleric, 3-methylbutyric (63); 2-methylbutyric (22); and butyric (24). Two alkanedioic acids frequently found were suberic, C_8 (87), and azelaic, C_9 (84). Three oxygen substituted acids were also identified with higher frequency: levulinic, C_5-4-keto

(267); 2-methoxy-4-methyl-2-pentenoic (299) and 2-methoxy-3-methyl-2-pentenoic (587). Possibly, the latter two compounds were actually present as the 2-keto species and were formed by methylation of the enol tantomer during diazomethane derivatization of the acid fraction.

- Eight aromatic carboxylic acids were identified in a majority of the concentrates: benzoic (17); ortho-, meta- and para-toluic (221, 72, and 73, respectively); 2,3-, 2,4-, and 3,5-dimethylbenzoic (189, 64, and 216, respectively); 2,4,6-trimethylbenzoic (219); phenylacetic (49); and phthalic (85).

- The most frequently identified water re-use indicators were salicylic (47) and clofibric (74) acids both of which are metabolites of the common high dosage drugs asprin and clofibrate (ethyl 2-(4-chlorophenoxy)-2-methylpropanoate), respectively. Other frequently identified water re-use indicators were nicotine (684), ethosuximide (298), BHT (1084) and oligomers of polyethylene and polypropylene glycol ethers. The latter compounds were not molecularly characterized in enough detail for entry in the computer managed database. However, they were always present in solvent extract type concentrates of DW which had vulnerable surface-water sources. The levels of these oligomeric materials were commensurate with the expected degree of re-use of the source water. These poly glycol compounds are commonly used in soaps, shampoos, cosmetics, ointments, paints and fabric softeners. Thus, it is not unexpected that they would be so commonly encountered, especially since they are known to be highly refractory toward biological or environmental degradation.

- Frequently identified compounds which can be classified as industrial solvents include: dichloroacetic acid (96), cyclohexanone (16), 2,5-hexanedione (202), isophorone (75), 3-methyl-2-cyclohexen-1-one (450) (similar to isophorone), 2,2,6-trimethylcyclohexanone (516), 3-methyl-2-cyclohexene-1-one (450), 3-hydroxy-3-methyl-2-butanone (427), diethylformamide (270), and lower molecular weight poly glycols such as propylene glycol methyl ether (45), diethylene-glycol butyl ether (79) and dipropylene glycol methyl ether (126).

- Frequently identified nonsolvent industrial compounds include acetophenone (67), p-dichlorobenzene (340), trichlorobenzene (354), and phenylacetonitrile (346). Most of the compounds which could be classified as chemical industry effluents were identified in too few concentrates for inclusion in this listing of frequently identified compounds.

- Other compounds frequently detected included common plasticizers such as di-n-butylphthalate (1), di-isobutylphthalate (20), diethylphthalate (37), and triethyl phosphate (97); the herbicides, 2,4-D (427). 2,4,5-T (190), and dicamba (112); bromodichloromethane (33), probably produced by chlorination at the waterworks; and phenol (156) and benzaldehyde (115) which could originate from a number of sources.

Special Interest Compounds--

Computer software (described in Appendix A) was developed to search the GC-MS data for the 53 compounds of Table 4. Results of the GC-MS data search are shown in Table 12. Also shown in Table 12 are other special interest compounds which were identified in the normal course of GC-MS data interpretation. These additional compounds are the semivolatile consent decree priority pollutants and the compounds on the EPA "Chemical Indicators of Industrial Pollution" list. The organization of Table 12 is parallel to Table 9 with both tables indicating specific search, consent decree and industrial indicator compounds with the symbols *, +, and $, respectively. In addition, quantification results in ng/l for the specific search compounds (not shown in Table 9) are shown in parentheses below the RS value entry in Table 12. Phthalates are listed separately in Table 12 to facilitate visualization of occurrence patterns for these high interest compounds. Clearly visible in the pattern of occurrences in Table 12 are the more frequent instances and higher levels for concentrates from Cincinnat, Philadelphia, and New Orleans which is consistent with expectations based on the source water. The relatively high number of specific search compound detection instances for S2C was principally attributed to higher sensitivity due to the very large volume sampled (11,750 liters), and the consistently lower RS values and concentrations shown in Table 12 are in agreement with this hypothesis. One noticeable aspect of Table 12 is the distinctly enhanced recoveries of these special interest compounds (except for the phthalates) shown for concentrate T1Y (direct XAD-2 extraction/diethylether elution) versus the concentrates T1C and T1X (RO pre-concentrated). This difference in recovery performance on identical water samples has been discussed in the sections covering these concentrates.

Some of the identifications of specific search compounds found in XAD-2 produced concentrates are in contradiction with expectations based on solvent extraction efficiencies: p-dichlorobenzene (S2X), 1,2,4-trichlorobenzene (S2X), fluoranthene (P2X and S2X), and diphenylamine (T4X). Note, however, that the detection of a moderately high level of aniline in concentrate T4X and the absence of this compound in concentrate T4C is not anomalous since none of the RO brine solvent extractions are performed at basic pH. There are 108 detection instances for the 31 specific search compounds shown in Table 12. The 7 most frequently detected compounds account for 50 (46 percent) of the 108 detection instances. These compounds (and the number of times detected) are: phenol (9), p-dichlorobenzene (8), styrene (7), pentachlorophenol (7), trichlorophenol (6), and fluoranthene (6 of which some may be as an artifact).

TABLE 12. SPECIAL INTEREST COMPOUNDS FOUND IN DW CONCENTRATES

Seq. No.[a]	Compound	Special Interest List[b]	Relative Size[c] of GC Peak for Detection in the Indicated Concentrate[d]																	
			V1C	V1X	T2B	T1C	T1X	T1Y	T4C	T4X	M2C	N2C	P2C	P2X	O2C	O2X	S2C	S2X	X1C	X1X
	COMPOUNDS ON THE SPECIFIC SEARCH LIST (TABLE 4)																			
			(Values in parentheses are ng per liter of original water)																	
36	2,4,6-Trichlorophenol	* + §	-2.0 (0.3)					6.0 (58)	3.6 (31)		0.6† (2.7)		4.8 (29)	-0.2 (0.8)			2.2 (1.6)			
130	Styrene	* §		0.0 (3.6)	1.0 (0.4)			5.0 (44)	-1.4† (0.8)				-0.2† (0.2)	0.3† (1.9)	3.9 (8.4)	0.9† (--)	0.2† (0.1)			
144	Hexachloro-1,3-butadiene	* + §						5.0 (1.6)				0.7 (2.7)								
156	Phenol	* +		2.0 (3.3)		5.0 (7.5)	4.0 (5.1)	3.0 (20)	3.6 (18)	3.6 (51)	2.6 (6.1)	3.7 (7.0)			0.9 (1.6)	3.9 (10)				
190	2,4,5-T	*				1.0 (4.8)		3.0 (31)	-0.4 (4.7)			3.7 (11)			4.9 (15)					
340	p-Dichlorobenzene	* + §			1.0 (0.1)	1.0 (0.3)		4.0 (86)	-0.4 (0.4)		1.6 (4.9)	3.7 (6.9)	-0.2 (0.2)				-0.8 (1.7)	2.2 (1.7)		
352	Pentachloroaniline	*						4.0 (8.2)												
354	1,2,4-Trichlorobenzene	* + §						4.0 (18)			1.6 (0.3)		-0.2 (0.2)				-0.8 (0.01)	2.2 (0.01)		
357	Pentachloronitrobenzene	*						4.0 (0.4)												
423	Pentachlorophenol	* + §	0.0 (0.2)			1.0 (1.0)		2.0 (4.1)	1.6† (2.6)			3.7 (0.6)		-0.2 (0.7)	3.9 (0.1)		1.2† (0.9)			
427	2,4-D	*				1.0 (2.3)		3.0 (28)	2.6 (44)			3.7 (54)			3.9 (4.3)	2.9 (--)				
468	p-Chlorophenol	* §				2.0 (0.5)		3.0 (45)	2.6 (46)				3.8 (0.6)		1.9 (3.1)					
471	2,4-Dichlorophenol	* + §							-0.4 (2.5)			2.7 (2.1)	3.8 (27)							
582	Aniline	*								3.6 (23)										
649	2,4-Dichloronaphthalene	*						3.0 (0.8)												
652	Nitrobenzene	* + §						3.0 (8.4)	-1.4 (3.3)											
810	Triphenyl phosphate	*										2.7 (0.1)								
817	o-Chlorotoluene	*						1.0 (2.0)	-0.4 (1.6)		2.6 (1.2)						-0.8 (0.1)	0.2 (0.2)		
871	o-Chloroaniline	*							-0.4 (1.6)	0.6 (3.9)							2.2 (3.1)			
882	Pentachlorobiphenyls	* + §															1.2 (--)	2.2 (0.3)		
933	Fluoranthene	* + §	-2.0 (0.3)					2.0 (0.9)	-0.4† (0.1)	-0.4 (0.1)	0.6† (0.3)			0.8 (3.7)				-0.8 (0.0)		
949	Lindane	* §						2.0 (0.8)				1.7 (0.4)					1.2 (1.5)	0.2 (0.8)		
1083	Diphenylamine	*								-0.4 (0.2)		1.7 (0.3)	-0.2 (0.1)				1.8 (0.2)	1.2 (0.01)		
1107	Heptachlor	* + §										1.7 (0.2)								
1165	Tetrachlorobiphenyl	* §						1.0 (--)												
1166	Pentachlorobiphenyl	* §						1.0 (0.4)												

TABLE 12. (continued)

Seq. No.[a]	Compound	Special Interest List[b]	Relative Size[c] of GC Peak for Detection in the Indicated Concentrate[d]																	
			V1C	V1X	T2B	T1C	T1X	T1Y	T4C	T4X	M2C	N2C	P2C	P2X	O2C	O2X	S2C	S2X	X1C	X1X
1248	Hexachlorobenzene	* + §										0.7 (0.3)	-0.2 (0.1)							
1255	p-Cresol	*	0.2 (0.01)	0.0 (0.2)					-0.4† (3.0)	-0.4† (9.9)										
1294	2-Methylstyrene	*							-0.4 (0.1)				-0.2 (0.1)				-0.8 (0.1)			
1301	2-Chloronaphthalene	* + §											-0.2 (0.01)							
1305	2,4-Dimethyl phenol	* +							-0.4 (2.8)	-0.4 (1.7)										
	COMPOUNDS NOT ON THE SPECIFIC SEARCH LIST																			
2	Naphthalene	+		5.1	1.0		5.0†		0.6	3.6†				7.8†	4.9	7.9†	2.2			2.2
62	Toluene	§			5.0					3.6			4.8			5.9		2.2	3.0	
75	Isophorone	+					3.0	1.0	2.6	2.7			5.8	3.8	1.9	3.9	1.2	2.2		
141	m-Xylene	§						5.0	0.6						1.9		2.2			
143	o-Dichlorobenzene	+ §						5.0			2.6		0.8		0.9		2.2			
157	1,1,2,2-Tetrachloroethane	§			5.0	5.0†	4.0†		0.6†		1.6†						0.2†	1.2†	5.0	
332	1,2-Dichloroethane	§				3.0		2.0								1.4				
335	Bischloroethyl ether	+ §		-1.0				4.0						0.8†		-0.1†				
417	p-Xylene	§			3.0			3.3†							1.9		1.2	2.2	4.0	
651	m-Dichlorobenzene	+ §						3.0					-0.2							
702	Phenanthrene	+	-1.0	3.0	1.0	1.0†	2.0†				0.6†	0.7†		2.8†		1.9†	0.2†	1.2†		-0.8
776	o-Xylene	§			2.0				0.6				2.8				2.2	2.2		
944	Fluorene	+						2.0												
995	Acenaphthalene	+							-0.4								-0.8		2.0	
1198	Pyrene	+			1.0									0.8†						
1203	Cumene	+			1.0				-1.4				0.8		0.9					
1213	n-Propylbenzene	§											-0.2		0.9		0.2			
1226	DDE	+ §										0.7		0.8						
	PHTHALIC ACID DIESTERS																			
1	Di-n-butyl phthalate	+ §	2.0	1.0	3.1	5.0		5.0		0.6†	8.7	8.3	8.1		4.0†		2.5†	1.2†		1.4
20	Di-isobutyl phthalate	§		1.0		5.0					6.6	6.0	3.8							
37	Di-ethyl phthalate	+ §			2.0	5.0	3.0	6.0	1.6†	3.6	4.6	4.7			3.9			1.2†	1.0	
76	n-Butyl isobutyl phthalate	§									5.6	3.7	5.8			2.9				
134	Dioctyl phthalate	+ §		3.0	2.0			5.0†				1.7†		2.8†						
245	Bis(2-ethylhexyl) phthalate	+ §	2.6			3.0†			4.6†		4.6†	4.7†	4.1†	2.3†	3.9†	4.0†				3.2
265	Dihexyl phthalate	+ §									4.6									
292	Butyl benzyl phthalate	+ §									4.6	3.7								
345	Dimethyl phthalate	§				4.0		4.0												
703	Dicyclohexyl phthalate	§	3.0						2.6†	0.6†						2.9†				
849	Di-n-propyl phthalate	§							2.6											

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a) The sequence number corresponds to the entry in Table 9.

b) The three special interest lists are coded: *: list of 53 compounds for which the GC-MS was specifically searched (see Table 4). +: list of "Consent Decree Priority Pollutants." §: list of "Chemical Indicators of Industrial Pollution" Federal Interim Primary Drinking Water Regulations (February 9 1978).

c) See Section 5, Analytical Scheme/Quantification of Identified Compounds for an explanation of the Relative Size Parameter.

d) See Tables 7 and 1 for translation of the three digit concentrate code names. The symbol, †, designates a detection instance that may be attributable to the concentrate generation blank.

Occurrence of Molecular Functional Groups in the Identified Compounds—

Associated with each identified compound entered in the computer-managed data base are a set of molecular functional group descriptors. A tabulation of the occurrences of the 25 functional groups in the DW concentrate results is presented in Tables 13 and 14. Percentages which each of the 25 functional group classes represent of the total number of identified compounds are shown in Table 13. Display of the percentage of the total parameter in Table 13 was chosen to facilitate comparison of the relative distribution of the functional groups among the analyzed concentrates. Thus, Table 13 provides comparative information on the numbers (but not the amounts) of compounds with the various function groups. Total RS values for each functional group are shown in Table 14, and this parameter reflects the amounts of material for each functional group (rather than the number of occurrences). Thus, these two tables are complimentary in the nature of the information provided. Note that the total number of identified compounds for each concentrate has been added to Table 13 to enable computation of the number of functional group occurrences from the percentages shown. Since these computer-printed tables (Tables 13 and 14) are generated from the data base before correction for the blank, the total number of identified compounds shown in Table 13 are also uncorrected for the blank. In the following discussion of Table 13, most of the conclusions are based on the results shown for the solvent extract concentrates since the values in the Table reflect a large contribution from XAD-2 resin bleed artifacts in concentrates T4X, M2X, N2X, P2X, and O2X.

Ten of the functional group types in Table 13 need no discussion due to a low or uniform distribution across the concentrates shown. These are: unsubstituted aliphatic, unsubstituted alicyclic, substituted alicyclic, halogenated PNA, substituted PNA, amide group, amine group, ether group, phenol group, and sulfur atom. Observations concerning the remaining 15 functional group types are the following:

- Halogenated species (aliphatic, alicyclic, and aromatic) have relatively higher detection frequency in three of the four surface waters most vulnerable to chemical industry pollution (T1C, T1Y, T4C, and N2C). M2C, which is not high, as expected, in halogenated aromatics is nevertheless high in halogenated aliphatics and halogenated alicyclics which probably results from chlorination of the high background of natural (humic-related) organic material in this concentrate. The average chloro compound frequencies for P2C is unexpected since the water source is similar to that for T1C/T1Y, T4C, and N2C.
- Comparing occurrence frequency values for the substituted aliphatic group with those for the substituted aromatic group shows that more of the nonhalogenated species were nonaromatic with the ratio of substituted aliphatic to substituted aromatic compounds averaging 1.6:1 for the solvent extract concentrates. The opposite, however, is true for

TABLE 13. OCCURRENCE OF MOLECULAR FUNCTIONAL GROUP TYPES IN DW CONCENTRATES, SHOWING THE NUMBER OF OCCURRENCES AS A PERCENTAGE OF THE TOTAL NUMBER OF IDENTIFIED COMPOUNDS

OCCURRENCE OF FUNCTIONAL GROUPS AMONG THE IDENTIFIED ORGANICS

PERCENT OF TOTAL*

		V1C	X1C	V1X	T2B	X1X	T1C	T1X	T1Y	T4C	T4X	M2C	M2X	N2C	N2X	P2C	P2X	O2C	O2X	S2C	S2X
1.	UNSUBSTITUTED ALIPHATIC	3	0	4	0	2	1	0	2	2	3	3	5	4	5	3	5	2	8	7	2
2.	HALOGENATED ALIPHATIC	0	4	1	0	0	7	3	12	7	2	9	2	6	3	5	1	2	2	5	6
3.	SUBSTITUTED ALIPHATIC	51	54	20	44	26	34	49	38	31	31	36	23	32	27	32	38	31	26	34	30
4.	UNSUSBSTITUTED ALICYCLIC	0	0	6	3	5	1	0	0	1	4	1	9	2	5	5	6	3	5	4	3
5.	HALOGENATED ALICYCLIC	0	0	0	0	0	0	0	2	1	1	2	0	3	0	1	0	1	0	1	3
6.	SUBSTITUTED ALICYCLIC	7	12	2	6	7	9	16	4	7	8	9	8	9	9	11	6	10	10	10	11
7.	UNSUBSTITUED AROMATIC	10	8	46	20	36	7	4	14	13	26	5	39	16	31	13	33	19	28	14	12
8.	HALOGENATED AROMATIC	7	0	3	1	0	7	4	21	9	2	4	2	10	5	5	3	3	2	5	5
9.	SUBSTITUTED AROMATIC	27	12	37	25	26	25	14	26	30	26	14	23	24	24	22	22	22	23	16	24
10.	UNSUBSTITUTED PNA	5	8	25	16	24	1	4	5	6	12	2	19	12	18	10	20	11	15	8	9
11.	HALOGENATED PNA	2	0	0	0	0	1	0	1	1	0	0	0	1	0	1	1	0	0	0	1
12.	SUBSTITUTED PNA	2	2	4	3	5	3	1	1	2	1	1	3	2	2	2	5	2	2	2	2
13.	ALCOHOL GROUP	22	25	13	16	10	19	38	10	21	16	25	13	14	12	21	15	12	13	21	16
14.	ALDEHYDE GROUP	2	2	4	3	3	1	1	1	1	5	3	3	0	5	3	3	5	3	3	4
15.	AMIDE GROUP	0	0	1	2	2	3	1	0	1	2	1	0	1	1	1	0	2	2	1	1
16.	AMINE GROUP	5	0	1	0	2	6	1	3	5	4	1	0	1	1	3	0	3	2	3	2
17.	CARBOXYLIC ACID	25	25	15	13	14	25	36	19	27	27	21	15	27	24	23	23	25	23	18	32
18.	ESTER GROUP	34	10	12	28	16	9	8	25	6	7	9	6	9	9	8	7	11	7	6	5
19.	ETHER GROUP	3	10	6	5	5	13	4	9	13	10	17	9	11	13	14	10	10	8	13	11
20.	HETEROATOM IN RING	7	12	2	3	5	16	3	2	10	5	11	4	5	6	8	1	9	7	8	5
21.	KETONE	8	15	13	4	7	15	18	8	12	15	15	19	14	15	15	13	18	21	22	16
22.	NITRO GROUP	2	2	2	1	0	1	3	3	4	2	0	0	2	0	0	0	0	0	1	2
23.	PHTHALIC DI-ESTER	10	2	3	3	3	3	1	2	2	2	3	1	4	1	1	1	1	1	0	1
24.	PHENOL GROUP	10	0	0	1	0	5	5	4	7	4	3	3	4	4	2	4	2	6	5	5
25.	SULFUR ATOM	3	0	1	1	0	2	0	2	1	1	0	0	1	0	2	0	1	0	1	1
	TOTAL NUMBER OF IDENTIFIED COMPOUNDS	50	52	158	99	58	151	77	243	193	181	220	239	249	233	292	221	233	231	289	171

* PERCENTAGE IS BASED ON THE TOTAL NUMBER OF IDENTIFIED COMPOUNDS RATHER THAN THE TOTAL NUMBER OF FUNCTIONAL GROUPS FORMED. THUS, THE SUM OF THE PERCENTAGES FOR A CONCENTRATE WILL TOTAL MORE THAN 100 PERCENT.

halogenated aromatics detected compared to halogenated aliphatics.

- Comparison of unsubstituted PNA, unsubstituted aromatic, and unsubstituted alicyclic values show the effect of XAD-2 resin bleed artifacts since most of these artifacts are classified in these three categories (compounds having only alkyl substitutents are considered unsubstituted in this work).
- The alcohol group does not show significant variation except for a lower value for concentrate T1Y (compared to T1C/T1X) in agreement with the earlier conclusion concerning the reduced effectiveness of the direct XAD-2 adsorption method for highly polar species.
- Consistently higher detection frequencies of the aldehyde group in the XAD-2 prepared concentrates is due to various alkyl benzaldehydes which may be present as a resin bleed artifact. Although it seems unreasonable that benzaldehydes would be present as a polystyrene impurity, air or peroxide oxidation at the styrene vinyl group could be responsible for these aldehydes.
- Except for two cases (T1Y and S2C) carboxylic acids were the most frequently encountered groups. For solvent extract concentrates, this functional group was present in an average of 23 percent of the compounds identified in solvent extract produced concentrates. Alcohols exceeded carboxylic acids in concentrate S2C; this result has already been discussed. For T1Y, carboxylic acids were exceeded in number by ester groups (see Below).
- The range of ester group detection frequencies varied little except for concentrate T1Y which, at 25 percent, was about 3-fold higher than the average for the solvent extract prepared concentrates. Most of these species were methyl and ethyl esters of both aromatic and non-aromatic acids. Since these results differ markedly from those for concentrates T1C and T1X (prepared from identical water), these esters must be suspected as artifacts. High levels of methanol and ethanol in the concentrate during storage could account for this anomalous result but should be discounted since the XAD-2 adsorption column was eluted with unpreserved, "distilled-in-glass" grade diethyl ether.
- The higher value of concentrate T1C for the heteroatom in ring group is the result of the large number of alkylated pyridines, quinolines, and isoquinolines found in that concentrate.

- Little variation in the frequency of detection of ketones was observed except for concentrate S2C. The relatively large number of ketones detected in this concentrate has been discussed earlier in Section 6. The relatively low value shown for T1Y as compared with T1C/T1X is in parallel with the similar observation for the alcohol group discussed above, and the same explanation applies in this case.
- The five Cincinnati concentrates show slightly higher frequencies for the nitro-group compared to other concentrates. This result is consistent with the observation that the Cincinnati concentrates contained more pronounced indications of chemical industry pollution than the other concentrates. The distinction, however, is not a marked one with respect to the Philadelphia concentrates.
- Phthalate diester identifications were slightly more in evidence in the Cincinnati, Miami, and New Orleans concentrates. It was surprising to find Miami included in and Philadelphia excluded from this group.

Since RS values span a logarithmic scale, the total RS value shown in Table 14 is not an arithmetic sum of the individual RS values since such a sum of logarithmic scale values would be mathematically related to the product of individual GC peak heights rather than the sum of them. For example, 10 GC-MS peaks, each with an RS value of 1.0 would give a total RS value of 3.0, and two peaks with RS values 2 and 8 would yield a total RS value of 8.0009. The mathematical basis of the GC-MS peak RS parameter is detailed in Section 5, Analytical Scheme. For the purposes of interpreting Table 14, it suffices that an an arithmetic difference of 1.0 between two total RS values in the table under comparison corresponds to a factor of one-half of an order of magnitude (3.16) change in the amount of material represented; a difference of 2.0 in total RS values corresponds to a factor of one order of magnitude (10.0), and so forth.

The DW concentrate functional group results expressed as total RS value for each classification category are shown in Table 14. These results are consistent with the conclusions made above concerning the frequency of occurrence of functional groups among the identified compounds as expressed in Table 13. The information in Table 14 allows some additional conclusions to be drawn concerning the relative amounts of organic material belonging to these classes of compounds. Again, attention is focused on the 7 solvent extract type concentrates plus concentrate T1Y since the amount of XAD-2 resin bleed artifacts in the XAD-2 resin produced concentrates does not allow a valid comparison. Concerning the type of molecular nucleus (i.e., the first 12 categories in Table 14) only three concentrates (M2C, N2C, and P2C) have the substituted aromatic nucleus representing the greatest amount of the identified organic material. However, after adjusting for the extremely high artifact levels of butyl phthalate in these concentrates, the substituted aliphatic nucleus assumes the highest ranking as for the other concentrates

TABLE 14. OCCURRENCE OF MOLECULAR FUNCTIONAL GROUP TYPES IN DW CONCENTRATES, SHOWING THE TOTAL GC PEAK SIZE FOR EACH GROUP ON BOTH GC COLUMNS

OCCURRENCE OF FUNCTIONAL GROUPS AMONG THE IDENTIFIED ORGANICS

TOTAL RS

		V1C	X1C	V1X	T2B	X1X	T1C	T1X	T1Y	T4C	T4X	M2C	M2X	N2C	N2X	P2C	P2X	O2C	O2X	S2C	S2X
1.	UNSUBSTITUTED ALIPHATIC	1.2	-	4.2	-	1.2	4.6	-	4.6	3.3	4.2	6.8	6.2	6.2	4.9	5.9	6.3	3.9	6.0	5.8	2.5
2.	HALOGENATED ALIPHATIC	-	2.2	-1.0	-	-	6.4	4.3	7.6	3.6	4.3	7.5	4.3	6.6	4.5	5.9	3.5	4.8	2.6	5.6	5.8
3.	SURSTITUTED ALIPHATIC	3.6	7.3	5.6	6.7	3.8	8.4	7.4	8.4	7.0	7.1	9.1	8.2	8.7	7.4	8.7	7.6	7.7	7.2	7.9	6.2
4.	UNSUSBSTITUTED ALICYCLIC	-	-	5.3	5.0	3.3	4.1	-	3.0	0.7	3.5	3.9	7.5	4.7	7.8	6.0	5.9	6.6	4.2	5.7	2.5
5.	HALOGENATED ALICYCLIC	-	-	-	-	-	-	-	4.4	1.6	1.6	5.2	-	5.1	-	3.1	-	2.5	-	2.1	3.7
6.	SUBSTITUTED ALICYCLIC	1.4	5.4	5.0	5.8	2.7	6.2	6.6	6.7	5.1	5.3	8.1	6.7	7.7	6.1	7.6	5.8	6.4	5.7	6.9	4.6
7.	UNSUBSTITUED AROMATIC	1.5	4.8	7.5	5.4	5.0	4.6	5.1	7.1	5.2	6.0	4.6	10.0	6.3	8.9	5.7	8.7	6.5	8.2	4.9	4.0
8.	HALOGENATED AROMATIC	0.5	-	3.3	1.0	-	5.4	5.1	7.4	5.1	5.7	5.8	4.1	6.3	5.6	6.2	4.0	5.8	3.9	4.6	4.1
9.	SUBSTITUTED AROMATIC	3.8	5.0	6.6	7.2	4.9	7.7	6.4	8.1	6.5	6.8	9.1	9.7	8.8	9.1	8.8	7.2	7.5	7.4	6.9	6.6
10.	UNSUBSTITUTED PNA	0.3	4.8	7.3	5.3	4.9	1.0	5.1	6.5	2.5	5.2	2.6	9.8	4.9	8.8	5.1	8.6	6.3	8.1	4.3	3.9
11.	HALOGENATED PNA	-1.0	-	-	-	-	2.6	-	3.1	1.6	-	-	1.6	2.8	-0.3	1.9	3.9	-	-	0.2	1.2
12.	SUBSTITUTED PNA	-1.0	4.0	5.4	5.0	2.5	3.5	4.0	5.8	3.2	3.9	5.6	6.8	5.0	5.1	5.2	6.2	5.1	5.0	3.8	3.5
13.	ALCOHOL GROUP	2.2	6.5	4.3	6.5	3.7	7.9	7.5	7.8	6.1	6.4	8.5	7.6	8.3	6.7	8.4	7.1	7.3	6.3	7.7	6.3
14.	ALDEHYDE GROUP	-1.0	6.0	4.7	2.6	1.6	4.3	4.0	5.5	3.9	4.7	6.0	6.9	4.7	5.9	5.7	5.7	5.4	4.6	5.5	2.1
15.	AMIDE GROUP	-	-	-1.0	2.6	0.2	5.4	4.0	2.0	3.2	4.0	5.3	-	5.4	4.8	3.9	3.8	5.7	3.6	3.4	1.2
16.	AMINE GROUP	1.2	-	8.0	-	0.2	4.8	3.0	5.4	3.4	4.4	2.7	3.6	5.8	3.0	3.3	8.8	4.2	3.5	4.4	2.1
17.	CARBOXYLIC ACID	2.3	6.1	4.7	5.4	4.5	8.4	7.0	7.8	7.3	7.5	8.8	7.9	8.5	7.5	8.4	6.8	7.9	7.5	7.4	7.1
18.	ESTER GROUP	4.0	4.9	5.0	7.2	4.1	7.2	4.1	7.7	5.4	4.6	8.9	7.5	8.7	6.5	8.4	6.0	6.2	5.9	6.3	3.6
19.	ETHER GROUP	2.2	4.9	5.3	5.2	3.3	7.6	6.2	7.0	5.7	6.4	7.9	7.1	7.3	6.3	8.0	6.7	7.2	5.8	7.3	5.6
20.	HETEROATOM IN RING	2.4	4.9	2.2	3.7	1.6	6.5	4.3	5.4	5.2	4.9	7.5	6.7	6.7	6.0	7.7	4.5	7.3	4.3	6.3	4.2
21.	KETONE	2.3	5.4	4.9	5.1	2.0	6.3	6.1	7.7	5.3	5.8	7.9	7.7	7.5	6.5	7.5	7.3	6.8	6.7	7.3	5.3
22.	NITRO GROUP	1.0	5.0	4.1	1.0	-	3.0	3.1	4.8	4.1	5.0	-	-	3.6	2.7	3.8	4.8	-	3.9	3.5	3.5
23.	PHTHALIC DI-ESTER	3.6	1.6	3.2	3.5	3.3	6.1	3.0	6.5	4.8	3.7	8.8	4.7	8.4	4.6	8.2	3.4	4.9	4.4	2.5	1.8
24.	PHENOL GROUP	1.4	-	3.1	1.0	-	6.5	4.8	6.8	5.0	5.6	5.5	6.4	6.4	5.5	6.0	4.7	4.7	5.7	5.4	6.0
25.	SULFUR ATOM	1.6	-	-1.8	2.8	-	3.8	-	6.6	2.6	2.6	-	3.6	5.3	2.7	4.8	-	3.6	-	3.5	3.8

and the substituted aromatic nucleus represented the second highest amount of material for these 8 concentrates. The high levels of chlorinated material in concentrates T1C, T1Y, T4C, M2C, N2C, and P2C is mirrored in the third (T1C and T1Y) and fourth (M2C, N2C, and P2C) highest ranking for the halogenated aliphatic nucleus and the fourth highest ranking (T1C, T1Y, T4C, and P2C) for the halogenated aromatic nucleus.

The quantitative rankings for substituent types (categories 13 to 25 in Table 14) shows acids and alcohols taking the highest and next highest rankings exclusively (5 concentrates show the acid group highest, 2 show it second highest, and P2C shows acids and alcohols at equal levels). The ether functional group ranked third highest in 5 (T1C, T4C, M2C, P2C, and S2C) of the 8 concentrates. In two cases, M2C and S2C, the levels of ethers and ketones were equal to this third highest level. This surprising level of ethers is due to poly glycols which were usually observed as major peaks, and, since these species usually have a terminal alcohol group, they undoubtedly contribute to the high (first or second) ranking for the alcohols noted above. Ketones and esters both ranked fifth for three concentrates (T4C, P2C and O2C; and M2C, N2C and S2C, respectively) with ketones ranking third once (N2C) and equal to ethers for third and fourth ranking in three concentrates (two with ethers, noted above, and one (T1Y) with esters). The fourth rank for the heteroatom in ring group in concentrate T1C was due to the large numbers of substituted pyridines, quinolines, and isoquinolines already discussed. The surprising second/third ranking of the heteroatom category for concentrate O2C is due to the high levels of dimethyl- and methylethylmaleic anhydrides and imides (four species) which were discussed earlier in the section covering that concentrate. Note that the high total RS values (8.8 to 8.2) for phthalic di-esters in concentrates M2C, N2C, and P2C were not considered in the preceeding discussion since they result principally from the high levels of dibutyl phthalate present in these concentrates as artifacts.

For the 7 solvent extract concentrates, the functional groups which represented the three lowest level categories were the following: nitro group, 6 concentrates (all but T4C); sulfur atom, 6 concentrates (all but P2C); amine group, 4 concentrates (T4C, M2C, P2C, and O2C); amide group, 3 concentrates (T4C, P2C, and S2C); aldehyde group, 2 concentrates (T1C and N2C); and phthalic diester, 1 concentrate (S2C). The main contributors to the sulfur atom total RS value were benzthiazole and benzenesulfonamides. Compounds contributing to the nitro-group total RS value were almost exclusively nitro aromatics. The nitro functional group is probably the most unambiguous indicator of chemical industry pollution of all the listed functional groups since it is the least likely to arise from natural organic material or the use of consumer products. In agreement with previous conclusions, the nitro group results of Table 14 indicate Cincinnati, Philadelphia, and New Orleans DW as containing more of these chemical industry indicators. The S2C total RS value (2.3) for the nitro group is due mostly to a questionable identification of 1-nitro-2-octanone at RS 2.2

Four additional functional group tables are presented in Volume 2. Three of these tables show the number of occurrences, the total RS parameter for SP1000 GC-MS analysis and the total RS parameter for SP2100 GC-MS analysis using a format identical to Tables 13 and 14. The fourth table shows all five parameters for each concentrate (i.e., those of Table 13 and Table 14 plus the other three cited above) in close proximity groupings for each concentrate to facilitate simultaneous comparison of all five parameters between concentrates.

The Effect of Concentrate Production Methodology on the Compound Identification Results--

The three types of concentrate production methodology used to produce the DW concentrates are described in some detail in Section 4. Two methods are based on sequential extraction of the RO brine in which solvent extraction of the brine is followed by XAD-2 adsorption and ethanol elution. Thus, two concentrates were prepared from each sampling. The third method (used to produce only one concentrate, T1Y) involved direct XAD-2 resin adsorption/diethyl ether elution without RO pre-concentration. Individual observations of the consistency of the identified compound results with chemical expectations based on the concentrate method are interspersed throughout the sections which discuss the results for each concentrate, and these will not be repeated here.

The following summarizes those observations:

- RO pre-concentration either allowed apolar species (such as substituted benzenes) to escape into the permeate water or absorbed them. The RO process was, however, apparently effective at recovering macromolecular materials (such as humic substances and poly glycols) ionic species (such as carboxylic acids) and highly polar species (such as alcohols, ketones, amides, ureas, sulfones, lactones, and others with similar polarity and/or hydrogen bonding capability).
- Solvent extraction of the RO brine removed most of the apolar and moderately polar species including the carboxylic acids which have normal acid strengths and lacked high polarity substitution. Since none of the solvent extractions were performed at strongly basic pH, strong bases were probably not recovered well. Humic species were also not recovered well but poly glycols were partially recovered.
- After solvent extraction, the RO brine contained the more water soluble species as evidenced by the compounds identified in the XAD-2 recovered concentrates. About 90 percent of the XAD-2 recovered organic material was humic substance. The identified compounds reported for XAD-2 generated concentrates were predominantly acids (especially dicarboxylics and polar-substituted acids) and the more polar substituted neutrals.

- Direct XAD-2 extraction apparently recovered apolar neutral compounds with greater efficiency than the methods based on RO preconcentration. However, the direct, acidic pH XAD-2 adsorption method performed less effectively than RO for the recovery of bases, highly polar neutrals (especially alcohols and ketones), higher strength acids (i.e., dicarboxylics and halo-aliphatic acids), humic substances and poly glycols.

One aspect of the concentrate production methodology which cannot be assessed with the information presently available is the adequacy of the performance toward strong bases. Aliphatic amines were so rarely identified in the concentrates that their few detection instances should perhaps be suspected as artifacts. In two cases (T1C and O2C), a variety of pyridines, quinolines, and isoquinolines were found. However, aniline, which is a specific search compound and, thus, could be detected with very high sensitivity, was identified in only one concentrate (T4X). Moreover, aniline-D_5 was one of the deuterated internal standards and its consistent recovery in the fractions and blanks indicates that basic compounds would have been detected had they been recovered in the concentrates at the 50 to 100 µg level (i.e., 30 to 60 ng/l for a 1500-liter sampling). Note that chloroanilines (mono through pentachloro species) were detected with some regularity, but these materials have such low base strengths that some of them are well extracted at acidic pH.

Another possible deficiency in the concentrate production methodology is suggested by the compound identification results for anhydrides, imides, lactones and lactames. Dimethylmaleic acid and methlyethylmaleic acids were identified at relatively high levels in all of the concentrates. The detection of the anhydrides of these acids as major constituents of the unpartitioned concentrate for O2C has been discussed earlier. These anhydrides were also found in other unpartitioned concentrates, but they could not have been present in the original water since they readily hydrolyze in the neutral pH range. A possible explanation is that dehydration of the free acid occurred during solvent evaporation steps of concentrate production, and this dehydration to the anhydride could have been enhanced by concomitant azeotropic water removal. Frequent detection of γ-lactones (2-furanones) and occasional detection of γ-lactames may also have been due to a similar dehydration of γ-hydroxy or γ-amino acids. These species hydrolyze less readily and, thus, could have partially escaped hydrolysis at the pH extremes of the partitioning scheme. The frequent detection of γ-hydroxy acids in the derivatized acid fraction may support this hypothesis. An alternative explanation is that these dehydrated species were formed during GC injection which, for the splitless GC-MS injection conditions, had durations of about 45 seconds. A definitive explanation of these observations would require additional experimental work.

Effect of the Raw Water Source on the Analysis Results—

Two samplings were of DW with a groundwater source (Poplarville, Mississippi, and Miami, Florida). As noted in Section 4, Poplarville was sampled because its source water (a deep aquifer) was extraordinarily organic-free and, thus, this sampling was appropriate as a field sample RO method blank (see Table 9 and the discussion of the Poplarville results earlier in this section). Just the opposite was the case for the Miami groundwater as noted in the earlier discussion of the M2C and M2X concentrate results. To summarize, one or more of the aquifers for raw Miami DW was, at the time of sampling, apparently vulnerable to intrusion of surface water with high levels of humic substances and was also vulnerable through the same or other routes to contamination with treated or untreated municipal wastes and/or solid waste leachate. Thus, the analysis results for these two DW samplings appear to span the entire water quality spectrum for groundwater sources and are not useful for making general inferences about groundwater DW sources.

In contrast to the lack of representative data for groundwater, above, the DW samplings with surfacewater sources provide an appropriate spectrum for comparison. Seattle represented source water with the lowest anthropogenic component of organic material but with a broad spectrum of natural organic materials expected from a conifer forested watershed. The concentrate analysis results were in agreement with reasonable expectations of the source water in a number of areas:

- Many of the identified compounds (alcohols and ketones) could have originated from natural degradation of oxygenated diterpenes which were also identified compounds of the concentrate
- There was minor evidence of the use of pesticides and herbicides but almost no evidence of water re-use indicators (i.e., those certain to have originated from domestic municipal wastes)
- The wide range of very low level hydrocarbons found were probably from air pollution in the Seattle metropolitan area which is transported and deposited as precipitation by the normal meteorologic patterns of the area
- The many non-aromatic chlorinated species observed probably were produced from naturally occurring organic material during chlorine disinfection and, thus, cannot be taken as representative of the source water although the high levels of these materials compared to the relatively lower levels of humic material may indicate unusually vigorous chlorination conditions at the treatment plant.

The Ottumwa, Iowa, and New Orleans, Louisiana, concentrates represent source surfacewaters with principally agricultural drainage components. Somewhat higher levels of materials reflecting water re-use and chemical industry effluents were expected and found in the New Orleans concentrates. However, concentrates from these two cities were the only ones in which the agricultural herbicide atrazine was found. Other herbicides and pesticides were also relatively predominant in the concentrates for these two cities. Significantly higher levels of humic-related material, as compared to the Seattle concentrates, was also in agreement with expectations based on the source water.

The Cincinnati, Ohio, and Philadelphia, Pennsylvania, concentrates represent surfacewater sources which are relatively more vulnerable to chemical industry effluents than those for Ottumwa and New Orleans. The higher levels and more numerous detection instances of compounds indicative of chemical industry effluent in concentrates from these two cities have been discussed earlier and can easily be visualized from the results shown in Table 12. Somewhat higher concentrations of typical water re-use indicators for these two cities compared to Ottumwa and New Orleans is in agreement with the higher population densities for the drainage basins in the former case.

Since Cincinnati was the only city for which the analyzed concentrates represented more than one sampling, the analysis results for those concentrates are the only ones which could reflect a potential effect of the sampling time of year. The first Cincinnati sampling (concentrates T1C, T1X, and T1Y) was performed on October 7, 1978, and the second sampling (T4C and T4X) was performed on January 14, 1980. The only aspect of the analysis results for these two concentrates which might be relevant to the time of year of the sampling is the apparently lower levels of humic-related material in the 1978 sampling as indicated by the residue weight analysis results shown in Table 7. The 1978 concentrate reflected a lower level of organic material (540 µg/l for T1C plus T1X compared to 860 µg/l for T4C plus T4X) and also gave a higher percentage of material recovered in the fractions (23 percent for T1C/T1X compared to 14 percent for T4C/T4X). The former result indicates higher concentration of humic substances in the 1980 water while the latter result indicates humic substances represented a lower fraction of the material in the concentrate for 1978. The observed effect is in opposition to that which would be expected based on the marked reduction in surface runoff in January due to the large percentages of frozen ground in the Ohio River drainage basin upstream from Cincinnati. No explanation of these apparently anomalous results can be offered at this time.

DISCUSSION OF AWT CONCENTRATE ANALYSIS RESULTS

Summaries of the Results for Each Sampling

All of the AWT plant samplings, for which discussions of the concentrate analysis results are presented individually below, were of a nominally 1500-liter (400-gallon) volume of finished AWT water taken on the plant site. In contrast to the DW concentrates, XAD-2 resin was not used to produce an additional extract of the RO brine. Instead, some of the six solvent extracts of the two RO brines produced (see Section 4) were analyzed separately or all six were combined for analysis as a composite concentrate. The third letter of the three-digit concentrate code name signifies the type of solvent extract:

Third Letter of Code Name	Concentrate Type
P	Pentane extract of cellulose acetate RO brine
M	Methylene chloride extract of cellulose acetate RO brine
N	Methylene chloride extract of cellulose acetate RO brine at pH 2
D	Methylene chloride extract of nylon RO brine at pH 2
C	Combination of all six solvent extractions of RO brine

A listing of the treatment steps for each AWT plant is given in Table 2 and complete descriptions of the plants have previously been reported (2). Thus, no further details of the AWT process for each plant is given in the discussion which follows.

Lake Tahoe, California,
October 24, 1974--

Four Lake Tahoe concentrates were analyzed; L2P, L2M, and L2N represent the cellulose acetate RO brine and L2D was produced from the nylon RO brine. L2D was the only extract of nylon RO brine analyzed separately from the cellulose acetate RO brine extracts.

The residue weight analysis results of Table 8 show that these four Lake Tahoe concentrates represented about 300 μg/l of organic material in the original water. The four-concentrate composited value for the overall recovery into fraction (81 percent) was the highest such value found. The values for concentration and percent recovery in fractions for the individual concentrates show some inconsistences:

- The level of 50 μg/l for L2D is surprisingly high since only material which permeated the cellulose acetate RO membrane can be recovered in concentrate L2D. Results for the DW concentrates T1C/T1X and T1Y indicated that highly apolar species can permeate the RO membranes. However, concentrate L2D should have contained only the most polar and acidic species remaining in the nylon RO brine after pentane and methylene chloride extraction, and there should have been only a small amount of these materials in the RO brine.

- Based on reasonable chemical expectations, concentrates L2M and L2N probably have reversed identities. Since L2N is an extract from acidic brine, a relatively higher amount of acids can be expected in it. In addition, since extraction of L2M preceded extraction of L2N, a higher relative amount of the high polarity species would be expected in concentrate L2M. The results for percentage recovery into fractions in Table 8 contradicts both of these expectations. The L2M versus L2N comparison also contradicts the corresponding values for fraction recovery for the Pomona concentrates C1M and C1N which are in agreement with the above stated chemical expectations.

Thirteen specific search compounds were found in the four Lake Tahoe concentrates (see Table 15): diphenylamine (L2P and L2M), pentachlorophenol (L2P and L2D), o-chloroaniline (L2P and L2D), phenol (L2M, L2N, and L2D), p-chlorophenol (L2M, L2N, and L2D), fluoranthene (L2P), styrene (all four concentrates), 2,4-dimethylphenol (L2D), crysene (L2P), 2-methylstyrene (L2M, L2N, and L2D), and hexachlorobenzene (L2N). Crysene was not detected in any other DW or AWT concentrate. In contrast to many concentrates, the four Lake Tahoe concentrates contained few chlorinated species (only 24 compounds after correction for the blank). The total number of compounds in Table 10 which have at least one detection instance for these four concentrates was 486. Since the sum of the numbers of identified compounds shown individually in Table 8 for each of the four concentrates is 647, it is clear that few compounds were identified in all or most of the four concentrates. Inspection of Table 10 shows that only 13 compounds were identified in all four concentrates and only 25 compounds were identified in any three concentrates. Certainly an appreciable degree of mutual exclusivity is expected between the classes of compounds that are extracted well by the two solvents, pentane and methylene chloride. A second factor which also has some effect is that the L2P, L2M, and L2N concentrates were the first three to be analyzed in this research program, and the GC-MS data interpretation activity for these three lacked the extensive experience that the analysts had gained with DW and AWT concentrates during the 22 month period preceding analysis of the L2D concentrate (34th in the series). In addition, the computer mass spectrum matching capability had been substantially improved in the interval between these analyses.

Most of the compounds identified in the acid fraction of L2P were fatty acids. Identification of pentachlorophenol at relatively high levels in L2P and at a low level in L2D but not in L2M or L2N was unexpected based on this compound's acid strength. Non-aromatic acids were more numerous than aromatic acids in L2M and L2N but the opposite was true for L2D. Clofibric acid was found at high levels in L2M, L2N, and L2D (in which it was the largest GC peak) and at lower levels in L2P. Ethosuximide, three barbituates, salicylic acid, and saccharin were also identified in some of the Lake Tahoe acid fractions.

In the aromatic fractions, 153, 10, 47, and 26 compounds were identified in L2P, L2M, L2N, and L2D, respectively. The large disparity for L2P was due to a high hydrocarbon component which was recovered from the RO brine essentially exclusively into the pentane extract. These compounds account for part of the lack of correspondence in identified compounds among the Lake Tahoe concentrates. Among these hydrocarbons were 15 compounds with fused ring systems larger than naphthalene, and this complement of polynuclear aromatic material constitutes the largest found for AWT and DW concentrates. Most of the identified compounds were alkylated benzenes, naphthalenes, tetralins, indenes, and indans. The RS values for these compounds ranged between 5 and 1, and 65 species had RS values of 3 or greater. Except for hexachlorobenzene, pentachloropyridine (both in L2N) and styrene and diphenylamine (both in L2M), the other aromatic fractions from the other three concentrates contained no compounds meriting discussion.

In the medium and high polarity fractions, poly glycols and phthalates (especially butyl phthalate) were the dominant species. L2P, as expected, contained almost no poly glycols, but the other three concentrates contained many of these oligomeric species at moderately high levels. RS values for these poly glycols ranged up to 7 for species identified sufficiently well enough for entry into the data base. Other AWT concentrates contained more or these materials by as much as an order of magnitude. Oxygenated diterpenes (17 species) were identified in L2P, L2M, and L2N, and these Lake Tahoe concentrates are unique among both the DW and AWT concentrates in this respect. Other compounds identified in the medium and high polarity fractions which may be of interest include caffeine (L2M, L2N, and L2D), nicotine (L2P and L2N), DMF (L2N), diethyl and dibutyl formamide (L2P), isophorone and two isomers of isophorone (L2N), 8 detection instances of alkyl phenols (for instance, nonylphenol), tris-2-chloroethylphosphate (L2M), and three polar anilines (chloro-, chloronitro, and nitroaniline, L2D).

Pomona, California,
September 25, 1974 (Pomona I)—

Three samplings were performed at the Pomona AWT plant. From the first sampling on September 25, 1974 (designated Pomona I), three of the RO brine solvent extract concentrates were analyzed: C1P, C1M, and C1N.

The composited residue weight results in Table 8 show that these three Pomona I concentrates (C1P, C1M, and C1N) represented the highest concentration (370 μg/l) of organic material in the original water of all the AWT composite concentrates or related sets of concentrates from a single sampling. The overall recovery of concentrate material into the analyzed fractions was 42 percent. This recovery value was about half that for the four Lake Tahoe concentrates (81 percent). The principal reason for the large difference between these two concentrates was the presence of a large amount of poly glycol materials in the Pomona I concentrates. On extraction of the RO brine, most of the poly glycols were apparently recovered in the pentane (C1P) and methylene chloride (C2M) concentrates. However, these moderately water soluble species are not recovered well through the fractionation scheme, and the lower recovery for C1P and C1M (compared to C1N) of concentrate material into the analyzed fractions is the result. The percentages shown in Table 8 for recoveries into fractions for the three Pomona I concentrates is completely consistent with chemical expectations based on the sequence of solvent extraction of the RO brine and the concentrate partitioning scheme.

A total of 348 different compounds (not counting compounds attributed to the blank) are listed in Table 10 as having been detected in concentrates C1P, C1M, and C1N, and 70 of these compounds (20 percent) were identified either in two of the concentrates or in all three. For comparison, only 25 of the 647 compounds (4 percent) identified in the four Lake Tahoe concentrates were identified in three or four of them.

As expected, the principal contributing factor to the lack of correespondence between the three concentrates in the identified compounds is attributable to the solvent extraction sequence. Concentrate C1P resulted in 77 identified compounds in the aromatic fraction while 34 and 56 compounds were identified in this fraction for C1M and C1N, respectively. Also, the acid fractions of concentrates C1M and C1N resulted in 84 and 63 identified compounds, respectively, while the C1P acid fraction yielded only 31 identified compounds. The Pomona I concentrates resutled in 31 identifications of chlorinated compounds and eleven of the 16 specific search compounds detected for C1P, C1M, and C1N were chlorinated compounds. The 16 specific search compounds which were detected for the Pomona I concentrates were: diphenlyamine, pentachlorophenol, phenol, styrene and 2-methylstyrene (detected in all three concentrates); 2-chloroaniline and fluoranthene (C1P and C1M); 4-chlorophenol (C1M and C1N); 2,4,6-trichlorophenol and 1,2,4-trichlorobenzene (C1P and C1N); 2,4-dichlorophenol and p-chloroacetophenone (C1M); and 2,4-D, hexachlorobenzene, and 1,4-dichlorobenzene (C1N). Detection of p-chloroacetophenone in C1M was the only detection instance for this compound in the DW and AWT concentrates.

In addition to the above listed specific search compounds, a number of noteworthy compounds were identified in the four analyzed fractions for these three concentrates:

- Acid fraction: four barbiturates (C1M plus phenobarbital, C1N), ethosuximide (C1M), salicylic acid (C1P and C1M), clofibric acid (C1P, C1M, and C1N), and saccharin (C1N) were the drug-related compounds identified. The relatively stronger acids, o-, m-, and p-chlorobenzoic three isomers of dichlorobenzoic, methylethylmaleic, and dichloroacetic acids, were identified in C1N. Methylethylmaleic acid was also identified in C1M.
- Aromatic fraction: most of the identified compounds were substituted benzenes and naphthalenes, with C1P containing more compounds and higher levels than C1M and C1N, as expected. Dichloroaniline (C1P), 3-chloroaniline (C1P), 2,4,6-trichloroaniline (C1N) and pentachloropyridine (C1N) were the nitrogen containing aromatics detected. C1P contained 6 species of polynuclear aromatic hydrocarbons (i.e., fused ring systems larger than naphthalene), but comparatively, these materials were at low levels.

- Medium and high polarity fractions: the most predominant components of the medium and high polarity fractions were poly glycol oligomers (noted above) which represented at least three distinct homologous series. Tris-2-chloroethyl phosphate was found at very high levels in C1M and somewhat lower levels in C1P and C1N, and the amount of this compound in the sampled water reflected by these three detections far surpassed amounts detected for any other sampling. Caffeine and dimethylsulfone were identified in concentrate C1N. DMF was identified in C1M and C1N. Benzonitrile, an aminomethylpyridine isomer, a trimethylpyridine isomer, and nicotine were also found in C1M. Large components of dioctyl phthalate and dioctylsebacate along with numerous fatty acid methylesters were identified in C1P.

Pomona, California,
October 2, 1974 (Pomona II)—

The only concentrate analyzed of the six RO brine extracts produced from the second Pomona sampling (Pomona II) was the methylene chloride extract of the acidified cellulose acetate brine (C2N). Concentrate C2N contained about half as much organic material, at 37 μg/l, as the other comparable Pomona concentrate (69 μg/l, C1N), Table 8. In addition, the overall recovery of C2N into the fractions was distinctly different from C1N at 20 and 88 percent for C2N and C1N, respectively. Compared to corresponding values in Table 8, the acid and aromatic fractions of C2N are apparently the source of this deviation. These two fractions and their corresponding blanks (but not the other fractions and blanks) inadvertantly evaporated to dryness during storage at -10°C before residue weights were determined. Thus, the comparative recovery differences in Table 8 for C2N are not considered significant.

The 106 compounds identified in concentrate C2N are listed in Table 10. Only 5 of those compounds contained chlorine. The 7 specific search compounds found in C2N are listed, with quantification results, in Table 15. The 7 compounds are: pentachlorophenol, 2,4,6-trichlorophenol, phenol, 2-methylstyrene, hexachlorobenzene, 1,4-dichlorobenzene and 1,2,4-trichlorobenzene. Only pentachlorophenol, at 11 μg/l, was found at a comparably high level. Consistent with other acidified brine methylene chloride extracts, relatively small amounts of the ubiquitous poly glycols and phthalate esters were identified. In addition to the results noted above, the analyzed fractions can be characterized as follows:

- Acid fraction: clofibric acid was the largest identified GC-MS peak (two other GC-MS peaks of comparable size could not be identified). Phthalic acid monobutyl ester was also a major component indicating that a large amount of dibutyl phthalate was probably present in the other (non-analyzed) Pomona II concentrates. The usual array of dicarboxylic acids, generally present at higher levels in acidified RO brine methylene chloride extracts than other extracts, were present, and 7 of these species were identified including the ubiquitous substituted maleic acids. Saccharin was also identified with an RS value of 5.

- Aromatic fraction: Only 11 compounds were identified, and most of these had RS values of 2 or less. The lack of appreciable material in this fraction is in agreement with all other results for brine extracts of this type. In addition to the specific search compounds listed above, the only noteworthy compounds identified were three phenyl substituted quinolines and isoquinolines two of which had RS values of 3.0.

- Medium polarity fraction: Most of the 24 compounds identified in this fraction had RS values of 2 or less, and, thus, this fraction was comparatively "clean". Three phthalates, benzaldehyde, benzthiazole, dimethylsulfone and DMF were also identified.

- High polarity fraction: The largest GC-MS peak was identified as tris-2-chloroethyl phosphate. This compound was also found at high levels in the Pomona I and Pomona III concentrates, but the level in C1M was distinctly higher than that for C1N. This result implies that the Pomona II concentrate produced by methylene chloride extraction of neutral pH RO brine (not analyzed in this work) may have contained even higher levels of this compounds than the level found in C2N. Other than 4 phthalate esters at moderately low levels, the only noteworthy compounds identified in this fraction were five non-aromatic nitrogen heterocyclics (piperidines,pyrimidines and pyrrolidines) none of which have confirmed identifications (see Table 10).

Pomona, California,
June 17, 1975 (Pomona III)--

All six solvent extracts of RO brines were combined for analysis as the composite concentrate, C3C. This concentrate represented only 87 μg/l of organic material in the sampled water and this amound is only 24 percent of the corresponding amount for the three Pomona I concentrates (Table 8). This rather large disparity between these two Pomona samplings is somewhat surprising. Consistent with the relatively lower amount of material present in concentrate C3C is the relatively low number of compounds (104) identified (see Table 10). Of these 104 compounds, 11 contained halogen and 9 were compounds on the 53-compound specific search list (Table 4). These 9 specific search compounds were: diphenylamine, 2,4,6-trichlorophenol, o-chloroaniline, phenol, tricresylphosphate (2 isomers), styrene, 2-methylstyrene and 1,4-dichlorobenzene. The levels for phenol, 2,4,6-trichlorophenol and 2-chloroaniline (39, 10 and 5 μg/l, respectively) were significantly higher than those for the other detections (see Table 15). The dominant characteristics of concentrate C3C were high levels of poly glycol oligomers and a high concentration of dibutyl phthalate. As visualized from the GC-MS chromatogram on SP2100 of the unpartitioned C3C concentrate, 60 to 80 percent of the concentrate material amenable to GC-MS analysis (before methylation of the acids) consisted of these high concentration materials. Although the separately analyzed concentrates (C1P, C1M and C1N) of Pomona I do not allow an exact comparison to this C3C chromatogram the separate chromatograms indicate that Pomona I was similar to Pomona III in the level of the poly glycol components. In addition to the compound identification results described above, the results for the four GC-MS analyzed fraction were as follows:

- Acid fraction: Surprisingly, clofibric acid was not identified in C3C although it was found at relatively high levels in all of the other Pomona I and Pomona II concentrates. 2,4,6-trichlorophenol, noted above, was one of the largest GC-MS peaks (RS value of 5) in this fraction. Many of the 34 compounds identified were acids containing phenyl substitution, and relatively fewer fatty acids were present. The largest identified GC-MS peak was phthalic acid monobutyl ester which was not unexpected based on the very large amount of dibutyl phthalate present in the concentrate.

- Aromatic fraction: The compound identification results for the aromatic fraction were similar to those for concentrate C1P except that most of the compounds were present at somewhat lower levels (i.e., 47 of the 56 compounds had RS values of 1.0). Most of the identified compounds were alkyl benzenes and naphthalenes. All three isomers of dichlorobenzene were identified (1,4-dichlorobenzene was noted above). Also present were 2,4,6-trichloroaniline and 1-chloro-3-nitro benzene (tentatively identified).

- Medium and high polarity fractions: These two fractions contained few identifiable compounds beyond the large complement of poly glycols and dibutyl phthalate. Only 7 compounds were identified in the medium polarity fraction, and only 2-chloroaniline (a search compound, noted above), 3-chloroaniline and 2,6-dimethylpyridine are noteworthy identifications. Only 16 compounds were identified in the high polarity fraction. In addition to the poly glycols and dibutylphthalate, a relatively high level of tris-2-chloroethyl phosphate was noteworthy. Similarly high levels of this compound, which is used as a flame retardant plasticizer and copolymer, were also found in the concentrates for Pomona I and Pomona II.

Orange County, California,
January 27, 1976—

The Orange County AWT plant, designated "Water Factory 21", which produced the sampled water has been the subject of a number of published studies on the development AWT techniques (10). All six solvent extracts of RO brines for this sampling were combined for analysis of the composite concentrate, R1C. This concentrate represented 104 μg/1 of organic material in the sampled water (see Table 8) and this value was in the middle of the range observed for AWT concentrates. The values in Table 8 for the recoveries into the fractions are somewhat diminished for the acid fraction and somewhat enhanced for the high polarity fraction compared to average values, but both are well within the wide ranges observed. The moderately high recovery in the high polarity fraction was principally the result of such an anomalously high level of dibutyl phthalate that it is nearly inconceivable that this compound was not present as an artifact. Inspection of the unpartitioned GC-MS chromatograms suggests that 50 to 70 percent of the organic material in the concentrate which was amenable to GC-MS analysis (before derivatization of the acids) was dibutyl phthalate. Other major constituents of these unpartitioned chromatograms were the plasticizers di-iso-octyladapate and di-iso-actylazelate and a lower than usual level of poly glycols. Overall, the R1C concentrate can be described as containing lower concentrations and fewer potentially noxious materials than most of the analyzed concentrates. In particular, it was nearly pristine in comparison to the Orange County II concentrate (R2C) which was prepared from a sampling taken only 6 days following that for R1C (see below). The lack of potentially noxious materials is underscored by the result that only one of the 53 specific search compounds was found in R1C (trichlorobiphenyl, 0.3 ng/l). Some possibly noteworthy findings from each of the analyzed fractions are the following:

- Acid fraction: Nearly every fatty acid from C_5 through C_{22} plus a number of isomeric fatty acids were detected. A number of benzoic acid species were also detected: methyl, dimethyl and trimethyl isomers plus 3-chlorobenzoic acid. Significantly, no phenolic compounds were identified, although some BHT and BHA related species were found in the medium and high polarity fractions, and trichlorophenol methyl ether was detected in the aromatic fraction.
- Aromatic fraction: Only 19 compounds were identified in the aromatic fraction and all but one of these had RS values of 2.0 or less. The identified compound with the highest RS value (3.0) was the methanoindene pesticide, nonachlor. An apparent octachloro analogue of nonachlor was also found but could not be identified as a specific molecular species. 2,4,5-Trichloroaniline, BHT, fluoranthene and fluorene were also identified, and most of the other species were substituted naphthalenes.
- Medium and high polarity fractions: Many of the compounds identified in these two fractions (26 and 42 compounds for the medium and high polarity fractions, respectively, were phthalates or poly glycols.

Some of the more interesting compounds which contained nitrogen or sulfur were: dimethyl, trimethyl and dimethyldihydroxy pyridines, trichloroaniline (also identified in the aromatic fraction), trimethyl-N-nitrosourea, cyclic maleic diamide, diethyl formamide, an isopropanolyl substituted isoxolidinone, N-butyl and N-methyl benzene sulfonamide, benzthiazole, isopropyl thiophene, tetrahydrothiophene dioxide (the solvent sulfolane) and dimethyl sulfone. Caffeine was the only drug or drug metabolite related material which was identified.

Some comparitive discussion of the analysis results for the Orange County I sampling (R1C) with those from the Orange County II sampling (R2C) can be found in the discussion, below, covering that concentrate.

Orange County, California,
February 3, 1976 (Orange County II)--

The Orange County II sampling was performed at the AWT plant, "Water Factory 21", only six days after the Orange County I sampling (R1C) which is addressed in the immediately preceding discussion. As for R1C, all six solvent extracts of RO brines from Orange County II were combined for analysis as the composite concentrate, R2C. This concentrate represented 144 μg or organic material in the sampled water (Table 8).

The distribution of concentrate material recovered into the fractions for R2C appears similar to that observed for R1C except that the values are uniformly higher. Upon closer inspection a somewhat curious result in the relationship between these concentrates becomes clear. The ratio, R2C:R1C, for the concentration value is 1.38. The corresponding values for the fractions are 1.36, 1.57, 3.6, and 1.32 for the acid, aromatic, medium polarity and high polarity fractions, respectively, and the ratio for the overall recoveries is 1.35. Thus, the difference between these two concentrates seems to be that the approximately 35 percent additional material in the R2C concentrate (compared to R1C) was not only all recovered into the fractions, but it was also distributed into them in a fashion such that the R2C fraction distribution was the same as that for R1C. A completely equivalent rationalization would be that R1C and R2C contained similar recoverable material but that R1C contained relatively less of it (and a correspondingly greater amount of unrecoverable material) than did R2C. There are, of course, many other possible explanations, but examination of the GC-MS chromatograms and the compound identification results (Table 10) indicate that there are, indeed, some distinct similarities in chemical makeup between these concentrates, as one might expect for samplings separated in time by only 6 days. Comparing the compound identification results (excluding those attributable to the blank) for R1C and R2C in Table 10 shows that 22 of the 59 compounds (37 percent) identified in both concentrates had larger RS values for R2C than for R1C while the reverse was true in only 12 instances (20 percent). Including the possible artifact compounds yields 32 of 71 (45 percent) detection instances with R2C RS values greater than those for R1C with 12 instances of the reverse (17 percent).

Certainly the most significant disparity between concentrates R1C and R2C is the number of identified compounds. Table 8 shows that 234 compounds were identified in R2C while only 106 were identified in R1C. This disparity is underscored by the specific search results (Tables 8 and 15) which show that 22 of the 53 search compounds were detected in R2C, but only one of them was detected in R1C. This detection of 22 compounds exceeded in number that for any other DW or AWT concentrate. The quantification results in Table 15 for these 22 search compounds shows that they were all detected at low levels relative to values shown for other AWT concentrates. 2,4,6-Trichlorophenol and 4-chlorophenol were both found at 9 ng/l, and 2,4-dichlorophenol, 2,4-D, and tricresylphosphate (2.4, 1.6 and 3.9 ng/l, respectively) were the only other compounds detected at greater than 1 ng/l. The other search compounds found were pentachlorophenol, 2-chloroaniline, fluoranthene, styrene, 2-methylstyrene, hexachlorobenzene, 1,4-dichlorobenzene, 1,2,4-trichlorobenzene, triphenylphosphate, 2,4,5-T, lindane, 2-chlorotoluene, heptachlor, tetra-, penta-, and hexachlorobiphenyls and DDT.

The chromatograms for these two concentrates were similar with the most noticable differences being distinctly higher levels of poly glycol compounds and lower levels of fatty acids (relative to aromatic acids) in R2C compared to R1C. Some of the other differences between the two concentrates involving specific compounds were:

- In the acid fraction of R2C, three often encountered water re-use indicators were identified: salicylic acid, pentabarbital and phenobarbital. These compounds were not identified in R1C. While nicotine was also found in R2C but not R1C, the opposite was true for caffeine

- More organophosphates were found in R2C than in R1C, and they were found in higher concentrations

- While a few alkyl-aromatics and halo-aromatics were found in the aromatic fraction of R1C, a considerably higher number of these compounds were found in R2C

- In the medium polarity fraction of R1C, three alkyl pyridines were identified. In contrast, the same fraction of R2C contained thirteen pyridine isomers (including pyridine) as well as four quinoline isomers.

Escondido, California,
July 8, 1975—

All six solvent extracts of RO brines for the Escondido sampling were combined for analysis as the composite concentrate, E1C. The values in Table 8 for residue weight analysis of concentrate E1C show that it represents one of the two lowest concentrations of organic material in the originally sampled water at 18 μg/l. The extremely low recovery (2.3 percent) into the acid fraction was a distinct departure from the results for other solvent extract composite concentrates. The only comparably low values were obtained for the pentane extracts (L2P and C1P) which would be expected to contain very few acidic species. Inspection of the GC-MS chromatograms of the unpartitioned concentrate reveals that most (80 to 90 percent) of the material amenable to GC-MS analysis (before derivatization of the acids) consisted of dibutylphthalate and numerous poly glycols oligomers. This result is in agreement with the recovery shown for the high polarity fraction (which represents 87 percent of the recovered material) since these materials appear in that fraction.

The 5 specific search compounds that were detected were all quantified at levels ranging from less than 0.1 ng/l to 0.6 ng/l (see Table 15). The five compounds were: pentachlorophenol, 2-chloroaniline, 4-chlorophenol, 2-chlorotoluene and 4-nitrophenol. In addition, E1C resulted in the fewest number of identified compounds (40, Table 8) and the lowest levels of these materials (aside from the butyl phthalate and poly glycols) of all the concentrates analyzed. The main features of the analyzed fractions were the following:

- Acid fraction: All but 3 of the 24 identified compounds had RS values of 3 or less. In addition to the specific search compounds, above, noteworthy identifications were (RS values shown in parentheses): clofibric acid (4.0), salicylic acid (3.0), phenobarbital (2.0), phenyldichloroacetic acid (2.0) and 4-chlorobenzoic acid (2.0)

- Aromatic fraction: There were so few sample constituents at detectable levels that the GC-MS chromatograms for this fraction were essentially indistinguishable from the blank, and the only compound identified was the specific search compound, 2-chlorotoluene, cited above

- Medium polarity fraction: 2,5-Hexanedione (RS 4.0), benzaldehyde (RS 3.0) and 2-chloroaniline (RS 1.0, a search compound, cited above) were the only noteworthy compounds among the 11 identified. Similarly to the aromatic fraction, the GC-MS chromatograms were nearly indistinguishable from the blanks

- High polarity fraction: Beyond the high levels of butyl phthalate and poly glycols, none of the 23 compounds identifies warrants discussion. Two isomers of chloroalkyl phosphates were found at moderately high levels, but these two species were not sufficiently well identified for entry into the data base.

The E1C concentrate was the only one of the AWT series for which the principal treatment phase of the AWT plant was the use of RO. The uniquely low level of acidic materials in E1C was not surprising since RO is expected to retain ionized species with high efficiency. However, the very high levels of butyl phthalate and poly glycols found in the concentrate seem inconsistent with correct performance of the RO unit and, thus, the possibility remains that these materials may have been present as artifacts.

Dallas, Texas,
November 11, 1974--

Only one of the six solvent extracts of the two RO brines produced from the Dallas sampling was analyzed. This concentrate, D2N, was the methylene chloride extract of the acidified cellulose acetate RO brine. The D2N concentrate represented 18 µg/l of organic material in the originally sampled water. Only the composite concentrate, E1C, contained organic material representing such a low concentration (see Table 8), although the two concentrates from Blue Plains I approached that level at 23 and 21 µg/l for B1M and B1N, respectively.

As expected for an extract from acidified RO brine, most (over half in this case) of the organic material was recovered in the acid fraction. In contrast to many of the other AWT concentrates, D2N contained relatively low levels of poly glycols and phthalates, and this result is reflected by the somewhat lower relative recovery in the high polarity fraction. This result was not unexpected, since most of the phthalates and poly glycols should have been removed from the RO brine during extraction with pentane and neutral methylene chloride which preceded D2N. The results for these solvent extracts of the Lake Tahoe and Pomona I samplings (L2P and C1P, respectively) are consistent with this prediction. Thus, the low levels of the nearly ubiquitous poly glycols and phthalates in D2N cannot be interpreted to mean that they were not present in the originally sampled AWT finished water.

Similarly to concentrate E1C, described above, concentrate D2N yielded relatively few identified compounds and low detected levels. While the number of identified compounds for D2N was about twice that for E1C, the total amount of material recovered into the fractions was higher by about a factor of three. The low levels of materials amenable to GC-MS analysis in D2N is further exemplified by the specific search results. Only two search compounds were found, and they were both at relatively low levels: 2,4-D and styrene at 1.6 and 1.4 ng/1, respectively (see Table 15). Not surprisingly, more than half of the compounds were identified in the acid fraction. The following summarizes the compound identification results for each fraction of concentrate D2N:

- Acid fraction: Of the 60 identified compounds, 44 had RS values of 3.0 or less. The largest number of identified compounds were saturated or unsaturated fatty acids with dimethyl and methylethyl maleic acids present at a relatively high level. Benzoic acid was among the components present at the highest levels, and a number of alkylbenzoic acids were also identified at substantially lower levels. All three isomers of chlorobenzoic acid (4-chlorobenzoic acid at RS 4.0 as well as 3,4-dichlorobenzoic acid were also detected. Salicylic acid and clofibric acid were also identified, but these were present at lower levels than usually encountered.

- Aromatic fraction: The GC-MS chromatograms for this fraction were nearly indistinguishable from the blanks. Although 19 compounds were identified, 16 of them had RS values of 1.0 or 0.0. Styrene (noted above), phenanthrene, (1,2-dichloroethyl)benzene (probably from chlorination of styrene), and 1,2-dichlorobenzene were among the identified compounds

- Medium polarity fraction: As for the aromatic fraction, the chromatograms for the medium polarity fraction were nearly indistinguishable from those for the blanks, and 11 of the 42 identified compounds had RS values of 1.0 or 0.0. BHT, di-t-butyl quinone, and dimethylsulfone were among the identified compounds

- High polarity fraction: Dibutyl phthalate (RS value 5.0) was the largest identified GC peak, and 26 of the 29 compounds had RS values of 3.0 or less. Other phthalates and plasticizers, fatty alcohols, DMF and tris-2-chloroethyl phosphate (RS value 3.0) were also identified.

The very low levels of organic material in the aromatic and medium polarity fractions, noted above, are not unexpected for a concentrate such as D2N produced by extraction of RO brine after prior extraction steps with pentane and methylene chloride.

Blue Plains, Washington, D.C.,
September 20, 1974 (Blue Plains I)—

Of the six solvent extracts of RO brine produced from the Blue Plains I sampling, only two were analyzed in this work: the methylene chloride extract of cellulose acetate RO brine, B1M, and the subsequent methylene chloride extract of the same RO brine after acidification, B1N. The Blue Plains I sampling is not related to the Blue Plains II sampling on May 31, 1975 (discussed separately, below) since these two samplings are associated with significantly different AWT schemes (see Table 2).

The B1M and B1N concentrates represent about the same amount of organic material in the original water at 23 and 21 µg/1, respectively, but the values for recovery of the concentrate materials into the fractions (Table 8) indicate some significant differences between these concentrates. B1N contained a greater relative amount of acidic material, as would be expected based on the acidic conditions under which it was extracted from the RO brine. B1M resulted in a lower overall recovery, and this result can be attributed to higher levels in this concentrate of poly glycols which are not recovered well through the fractionation scheme. This effect has been observed for other similar concentrate pairs (i.e., C1M and C1N) and is supported by the GC-MS analysis results which show relatively higher amounts of these poly glycol materials in the unpartitioned concentrate and high polarity fraction for B1M as compared to B1N.

Although the values for residue weight analysis in Table 8 indicate that there are some significant differences between B1M and B1N, there are far more similarities than differences with respect to the nature of the organic material amenable to GC-MS analysis. This result can be seen both in the compound identification results and in some distinct similarities between the corresponding chromatograms for these two concentrates for the acid and high polarity fractions. Comparison of the compound identification results in Table 10 for B1M and B1N shows that 47 of the 177 compounds (27 percent) were identified in both concentrates. For comparison, the corresponding value for the concentrates C1M and C1N was 17 percent.

The relative similarity in the identified compounds for B1M and B1N is also demonstrated in the specific search compound results. Of the 7 search compounds identified, 4 were identified in both B1M and B1N: pentachlorophenol, phenol, p-cresol and 2,4-dimethylphenol (found in both concentrates); fluoranthene and hexachlorobenzene (B1M); and 2,4-dichloronaphthalene (B1N). The quantitative results for these 7 compounds are presented in Table 15. Examination of the compound identification results of Table 10 shows that most of the disparities in the results for B1M and B1N are consistent with expectations based on the sequence of the extraction from the brine (B1M was extracted first) and the pH of the extraction (unbuffered for B1M and acidic for B1N).

Some of the features of the compound identification results which may be of interest are listed below:

B1M:

- Acid fraction: Normal and isomeric fatty acids were the largest group of compounds identified. Clofibric and salicylic acids were identified at moderate levels. Methylethylmaleic and dimethylmaleic acids were present at relatively high levels along with the related compound, methylethylmaleamide. Phenol and five alkylated phenols were detected with all three isomers of cresol found at unusually high levels. Other noteworthy compounds include:

2-aminobenzoic acid, 2-amino-5-chlorobenzoic acid, p-aminophenylacetic acid and 2,4-dichlorobenzoic acid. There were relatively few halogenated compounds identified in the acid fraction.

- Aromatic fraction: Only 12 compounds, all at relatively low levels, were detected, including hexachlorobenzene, fluoranthene, acenaphthalene and 2-methylnaphthalene.
- Medium polarity fraction: Of 22 compounds, 19 had RS values of 3 or less. Terpin, diethylcarbonate, dimethylsulfone, acetamide and quinoline were identified.
- High polarity fraction: Tris-2-chloroethylphosphate was found at relatively high levels. Many species of plasticizers (phthalates and others) and poly glycols were identified at moderately high levels.

B1N:

- Acid fraction: The predominant species identified were nonaromatic carboxylic acids (18 unsubstituted fatty acids and 10 unsaturated and/or keto and methoxy fatty acids). Palmitic, oleic, linoleic and linolinic acids were the four largest GC peaks. The typical aromatic acids were also present: benzoic, phenylacetic, salicylic, phthalic and 2,4-dichlorobenzoic acids. The amino and amino-halo aromatic acids identified in B1M were not detected. However, six halo-substituted and, therefore, relatively stronger acids were identified which were not seen in B1M: chloroacetic, 2,2-dichloropropanoic, 2,2-dichlorobutanoic, trichloroacrylic, 4,4-dichloro-2-butenoic and 4-chloro-2-butenoic acids.
- Aromatic and medium polarity fractions: These two fractions contained almost no material at all. The highest level compounds of the medium polarity fraction were ketones, some of which remain unidentified but are probably diterpene related. A number of lactones were also found (N-methyldelta; N-methyl-gamma; delta; and epsilon).
- High polarity fraction: The usual di-ester plasticizers and polyglyols were identified, but these were present at distinctly lower levels than for B1M. A relatively large number of gamma-lactones, furans, and other cyclic and/or unsaturated ketones were also detected as well as the natural product terpin. Tris-chloroethyl phosphate was also identified but at a far lower level than for B1M.

Blue Plains, Washington, D.C.,
May 31, 1975 (Blue Plains II)--

All six solvent extracts of RO brines for the Blue Plains II sampling were combined for analysis of the composite concentrate, B2C. An earlier sampling at this AWT plant (Blue Plains I, B1M and B1N, see previous discussion section) was concerned with a different treatment plant sequence, and, thus, is not related to concentrate B2C. The 46 μg/l of organic material which the B2C concentrate represented in the originally sampled water was comparable to the corresponding composite value (44 μg/l for concentrates B1M and B1N (Table 8). However, the distribution of recoveries of the organic material into the fractions was substantially different for B2C compared to B1M/B1N with the B2C acid fraction recovery equal to about one fifth of that for B1M/B1N and the high polarity fraction recovery for B2C higher by more than three times that for B1M/B1N. The very high levels of dibutyl phthalate and poly glycols present in B2C easily account for the predominance of the high polarity fraction among the others. This results is graphically illustrated by the strong similarities in appearance of the high polarity fraction chromatograms with those for the unpartitioned concentrate. The chromatograms of the unpartitioned concentrate suggest that these anomalously high levels of phthalate and poly glycols account for 70 to 90 percent of the organic material in the concentrate which was amenable to GC-MS analysis (before derivatization of the acids).

Six of the specific search compounds were found in concentrate B2C: pentachlorophenol, 2,4,6-trichlorophenol, tricresyl phosphate, p-cresol and styrene. Tricresyl phosphate was quantified at 130 ng/l, and this was the highest level determined for all search compound detections in both DW and AWT concentrates. The presence of p-cresol in B2C may be related to the high level of tricresyl phosphate as a hydrolysis degradation product of tricresyl phosphate either before or after preparation of the concentrate. This hypothesis may be supported by the detection of o-cresol and m-cresol at levels similar to those for the search compound, p-cresol.

In addition to the distinguishing feature of the tricresyl phosphate, was the detection of a number of chlorinated and brominated species in the acid fraction (described below). This array of halo-acids was unique among the AWT concentrates analyzed. The main characteristics of the analyzed fractions were the following:

- Acid fraction: Significantly more compounds (83) were identified in the acid fraction than in the other three fractions. The most predominant materials were fatty acids, benzoic acid, and phenyl substituted aliphatic acids. There were a surprising number of bromo, chloro, and bromochlorobenzoic acids and phenols detected: chlorobenzoic, dichlorobenzoic, bromochlorobenzoic, bromobenzoic and dibromobenzoic acids were identified as well as dichlorophenol, trichlorphenol, pentachlorophenol, and tribromophenol. Moreover, an additional 8 bromo, 3 chloro, and 2 bromochloro compounds were detected but it was not possible to identify these compounds with enough specificity to enable entry in the data base.

- Aromatic fraction: This fraction contained so few compounds that the chromatograms were nearly indistinguishable from the blank. The only two compounds identified were trichloroaniline and bromochloroaniline

- Medium polarity fraction: Dibutyl phthalate was the only compound of the 18 identified that had an RS value greater than 3.0, and 16 of these 18 compounds had RS values of 2.0 and 1.0. Phenylacetonitrile and di-t-butyl quinone were the only noteworthy compounds found

- High polarity fraction: Phthalates and poly glycols were the compounds identified at the highest levels in this fraction. Tricresyl phosphate, discussed above was the only other noteworthy compound identified.

Comparison and Discussion of AWT Concentrate Analysis Results

The degree to which the GC-MS Analysis Results Characterize the Sampled AWT Water--

The degree to which the compound identification results correctly reflect the organic material present in the sampled water is principally dependent on three factors: 1. The completeness of recovery of organic material from the sampled water, 2. The completeness of recovery of the concentrate material into the analyzed fractions and, 3. The percentage of the material recovered in fractions which can be successfully analyzed by GC-MS. The effect of each of these factors is addressed in the discussion below.

In contrast to the DW samplings, extraction of the AWT RO brines with XAD-2 resin was not performed following the solvent extractions. Thus, no conclusions can be made concerning the nature of the organic material not recovered from the AWT RO brines. However, it can be concluded that most of the organic material present in the sampled AWT water was not recovered in the concentrates. Some of the factors which relate to this conclusion are the following:

- TOC values in Tables 1 and 2 indicate that the sampled AWT water contained distinctly more organic material (by factors ranging from 2 to 10) than the sampled DW

- The concentrations which the DW and AWT concentrate material represented in the sampled water (Tables 7 and 8, respectively) were, on the average, significantly lower for AWT solvent extract concentrates than for this type of DW concentrate

- In the corresponding section of the discussion covering the DW concentrates the conclusion was made (based on the amounts of material in solvent extract and XAD-2 extract concentrate pairs) that only 15 to 25 percent of the organic material contained in the RO brine was recoverable by solvent extraction.

Thus, an even lower fraction of the organic material present in the sampled AWT water was recovered into the AWT concentrate than was recovered from the DW source water into the DW solvent extract type concentrates. Taking 6 mg of carbon per liter as a typical TOC value for AWT water, 0.6 as an approximate weight fraction that carbon represents in the organic material, and 100 µg/l as a representative value for the concentration of organic material in the original water represented by an AWT concentrate, the calculated result is that the organic concentrate represents only 1 percent of the organic material in the sampled water.

In comparison of the values for overall recovery of AWT concentrate material into the fractions (Table 8), no pattern emerges which is dependent on the type of concentrate or the source of the sampled water. The range of total percent recovery values for composited extract concentrates and the composited values for the sets of individually analyzed extract concentrates (Lake Tahoe, Pomona I and Blue Plains I) ranged from 23 percent for concentrate E1C to 81 percent for the four Lake Tahoe concentrates. The presence of high levels of poly glycol oligomers has been found to reduce overall recoveries. This reduction has been attributed to the water solubility of these materials and their partial loss during aqueous/organic partitioning steps of the fractionation scheme. Only the concentrates representing Blue Plains I (B1M and B1N) and Lake Tahoe (L2P, L2M, L2N and L2D) contained low amounts of these poly glycols, and the recovery values for these two concentrates were at the upper range of the values found (60 and 81 percent for Blue Plains I and Lake Tahoe, respectively). In contrast, all of the poly glycol dominated composite concentrates or sets of concentrates except one (B2C) had overall recoveries which were lower than the Lake Tahoe and Blue Plains I values but the percentage recoveries did not correlate well with the relative amounts of poly glycol material present. In the case of DW concentrates, low recovery into fractions usually correlated with the presence of high levels of humic material, and this condition was always apparent in the GC-MS data for the acid fraction as a broad, late eluting profile of unresolved peaks in the chromatogram. No comparable results were observed for the AWT concentrates which could be correlated with the results for overall recovery into the fractions. Thus, the extent to which the presence of humic material effected recoveries of AWT concentrate material into fractions cannot be assessed. Certainly, there are other classes of organic material in the concentrates which are not recovered well in the concentrate fractionation scheme, and the relative levels of these probably varied widely among the concentrates depending on variations in the AWT plant feed water and differences in the treatment modules used at each plant. Thus, the data presently available do not permit speculation on the nature of the AWT concentrate material which was not recovered in the fractions except that for certain concentrates, part of that material was probably poly glycols.

It is not possible to unambiguously determine what portion of the AWT concentrate fractions was amenable to GC-MS analysis. However, based on the types of compounds identified, the residue weight results and their correspondence to GC-MS chromatographic profiles, and the residues left on the GC injector liner following sample injection, the acid fraction was the only fraction which contained appreciable but highly variable amounts of material which was not amenable to GC-MS analysis. In contrast to the DW concentrates, no pattern was observed for the AWT concentrates, and the relative amounts of material recovered in the fractions which was not represented in the compound identification results can be estimated to range from a small portion for some concentrates to less than about one half for certain concentrates containing high levels of acidic material (B1N, D2N, C1N and possibly L2N).

Compounds Identified in most of the AWT Concentrates--

Table 10 conveniently displays the frequency with which compounds were detected in the AWT concentrates. As expected, the most frequently detected compounds are located near the beginning of Table 10. The 16 AWT concentrates for which Table 10 presents the identified compound results were produced from 10 samplings, as noted in Table 8. For 991 of the 1107 compounds shown in Table 10, more than half of the detection instances among the 16 AWT concentrates were not attributable to the blank. The number of compounds for which detection instances not attributable to the blank were shown for 5 or more of the 10 samplings was 65, and, except for 4 compounds, they appear among the first 390 compounds in Table 10. These 65 frequently identified compounds can be taken as indicative of the average chemical profile of the AWT concentrates, and they are listed below by catagories with the entry sequence number of each compound in parentheses:

- Methylethyl maleic acid (17) and dimethyl maleic acid (50) were not successfully identified until after the completion of analysis of concentrates L2P, L2M, L2N, C3C and C1P. Thus, these two compounds are not shown as having been detected in those concentrates. Inspection of some of the acid fraction chromatograms shows these compounds probably were present in a few cases. This result is not surprising since these compounds were detected in most of the other AWT and all of the DW concentrates. These compounds are monomers used in polyester (alkyd) resins used in paints and other polymer applications, so their nearly ubiquitous detection is not surprising

- Although many of the longer chain (C_{10} to C_{18}) fatty acids in Table 10 have been designated as attributable to the blank, 9 shorter chain fatty acids qualify for listing here: valeric, C_5 (204); 2-methylbutyric (202); caproic, C_6 (71); 2,2-dimethylbutyric (102); n-heptanoic (120); caprylic, C_8 (33); 2-ethylhexanoic (9); and the alkane diacid, subereric, C_8 (91)

- Of the 13 acids containing a phenyl moiety, most were substituted benzoic acids: benzoic (10); o-, m-, and p-toluic (30, 15 and 43, respectively); 2,4-, 2,5- and 3,5-dimethylbenzoic (12, 37 and 42, respectively); 2,4,5-trimethylbenzoic (125); o-, m- and p-chlorobenzoic (53, 123 and 44, respectively); phenyl acetic (36); 2-phenylbutyric (100); phthalic (111) and monobutyl phthalic (36). The frequent detection of monobutyl phthalic acid should probably be disregarded since it correlated with the detection of very high levels of dibutyl phthalate which was suspected as an artifact. Phenol (208) and p-chlorophenol (209) also qualify as frequently detected compounds. Other phenols, in particular the chlorinated phenol search compounds, were also frequently detected, but, due to low RS values, most detection instances were attributed to the blank (see the discussion concerning the specific search results, following section).

- The list of frequently detected plasticizers was dominated by phthalates: dibutyl (3), dioctyl (8), methyl butyl (57), di-isobutyl (81), n-butyl-isobutyl (94) and dimethyl (197). Di-isobutyl and n-butyl-isobutyl phthalates probably would not have been classified as frequently detected if the very high levels of di-n-butyl phthalate had not been present (see above). The fire retardant plasticizer, tris-2-chloroethyl phosphate (13) was also frequently detected at high levels.

- Glycol ethers and poly glycol oligomers were frequently detected, and 9 species (sequence numbers: 4, 11, 18, 19, 21, 61, 63, 148, and 371) detected in more than half the samplings.

- 6 Compounds can be classified as organic solvents although some may have other industrial uses: n-butanol (22), 3-hexanol (214), benzyl alcohol (268), 2-cyclohexanone (369), 2,5-hexanedione (370) and dimethyl sulfone (387).

- 7 Aromatic hydrocarbons, generally found at low levels, may be due to the presence of fuel oil or other petroleum distillates in the original water: psendocumene (337), naphthalene (92), 1-methylnaphthalene (517), 2-methylnaphthalene (340), 1,6-dimethyl-4-isopropylnaphthalene (566), biphenyl (346) and fluorene (753).

- 5 Compounds were possibly attributable as chemical industry effluents: benzoldehyde (160), n-butylbenzene sulfonamide (131), 2-chloroaniline (186), styrene (334) and 2-methylstyrene (802).

- Not surprisingly, 5 domestic sewage indicators were found among the frequently identified compounds: clofibric acid (1), salicylic acid (110), ethosuximide (39), phenobarbital (101) and BHT (34).

Special Interest Compounds--

Computer software (described in Appendix A) was developed to search the GC-MS data for the 53 compounds of Table 4. Results of the GC-MS data search for the AWT concentrates are shown in Table 15. Also shown in Table 15 are other special interest compounds which were identified in the normal course of GC-MS data interpretation. These additional compounds are the semivolatile consent decree priority pollutants and the compounds on the EPA "Chemical Indicators of Industrial Pollution" list. The organization of Table 15 is parallel to Table 10 with both tables indicating specific search, consent decree and industrial indicator compounds with the symbols *, +, and $, respectively. In addition, quantification results in ng/l for the specific

TABLE 15. SPECIAL INTEREST COMPOUNDS FOUND IN AWT CONCENTRATES

Seq. No.[a]	Compound	Special Interest List[b]	Relative Size[c] of GC Peak for Detection in the Indicated Concentrate[d]																	
			V1C	X1C	L2P	L2M	L2N	L2D	C3C	C1P	C1M	C1N	C2N	R1C	R2C	E1C	D2N	E2C	B1M	B1N
	COMPOUNDS ON THE SPECIFIC SEARCH LIST (TABLE 4)																			
			(Values in parentheses are ng per liter of original water)																	
7	Diphenylamine	*			5.2 (1.5)	1.6 (0.01)			1.0 (0.1)	8.0 (9.8)	3.1 (2.2)	2.0 (0.1)								
162	Pentachlorophenol	* + $	0.0 (0.2)		5.0 (17)			1.0† (5.2)		4.0† (44)	4.0† (10)	4.0† (6.8)	5.0 (11)		1.0† (0.1)	1.0† (0.0)		1.0† (0.7)	1.0† (0.2)	1.0† (0.4)
163	2,4,6-Trichlorophenol	* + $	-0.2 (0.3)					1.0† (3.9)	5.0 (9.6)	3.0 (1.6)		2.0† (2.4)	4.0 (1.3)		4.0 (9.1)			1.0† (0.2)		
186	o-chloroaniline	*			3.2 (0.6)			2.0 (2.7)	2.0 (4.5)	3.0 (3.9)	5.0 (25)				1.0 (1.0)	1.0 (0.6)				
208	Phenol	* +				4.0 (1.1)	4.0 (8.5)	5.0 (23)	3.0 (39)	2.0 (4.8)	5.0 (20)	5.0 (11)	5.0 (4.6)					3.0 (3.6)	3.0 (0.6)	3.0 (6.7)
209	p-Chlqrophenol	* $				1.0 (1.6)	1.0 (8.1)	3.0 (100)			5.0 (16)	4.0 (55)			1.0 (9.0)	2.0 (0.3)				
250	Tricresyl phosphate	*							2.0 (1.7)						1.0 (3.9)			5.0 (130)		
270	2,4-D	*										5.0 (70)			1.0 (1.6)		2.0 (1.6)			
308	p-Cresol	*	0.2 (0.01)															4.2† (16)	4.0† (79)	3.0† (49)
322	Fluoranthene	* + $	-2.0 (0.3)		1.0† (0.2)					4.0 (3.4)	1.0† (0.2)				2.0† (0.8)				1.0† (0.9)	
334	Styrene	* $			4.0 (0.9)	2.0 (1.0)	1.0 (0.4)	0.0 (—)	1.0 (0.8)	2.0 (0.7)	1.0 (1.4)	2.0 (0.6)			1.0 (0.5)		1.0 (1.4)			
422	2,4-Dichlorophenol	* + $									4.0 (—)				1.0 (2.4)			1.0 (0.8)		
591	2,4-Dimethylphenol	* +						1.0 (2.0)											3.0 (8.9)	1.0 (1.0)
775	Chrysene	* +			2.0 (5.1)															
802	2-Methyl styrene	*				1.0 (0.01)	1.0 (0.6)	1.0 (0.1)	1.0 (0.1)	1.0 (0.6)	2.0 (0.6)	1.0 (0.3)	1.0 (0.1)		1.0 (0.1)					
821	Hexachlorobenzene	* + $					1.0 (0.1)					2.0 (3.4)	1.0 (1.6)		1.0 (0.6)				1.0 (0.7)	
834	p-Dichlorobenzene	* + $							1.0 (0.01)			2.0 (0.6)			1.0 (0.2)					
836	Tri-m-cresyl phosphate	*							2.0 (0.8)											
840	1,2,4-Trichlorobenzene	* + $								2.0 (0.7)		1.0 (0.1)			1.0 (0.1)					
996	N-nitroaniline	*						1.0 (0.5)												
1014	Triphenylphosphate	*								1.0 (1.3)					1.0 (3.4)					
1017	p-Chloroacetophenone	*									1.0 (7.5)									
1034	2,4,5-T	*													1.0 (0.5)					
1035	Trichlorobiphenyl	*												1.0 (0.3)						

(continued)

TABLE 15. (Continued)

Seq. No.^{a}	Compound	Special Interest List^b	Relative Size^c of GC Peak for Detection in the Indicated Concentrate^d																	
			V1C	X1C	L2P	L2M	L2N	L2D	C3C	C1P	C1M	C1N	C2N	R1C	R2C	E1C	D2N	B2C	B1M	B1N
1037	Lindane	* $																		
1038	o-Chlorotoluene	*													1.0 (0.2)					
1039	Heptachlor	* + $													1.0 (0.2)	1.0 (0.2)				
1040	Tetrachlorobiphenyl	* + $													1.0 (0.5)					
1041	Pentachlorobiphenyl	* + $													1.0 (0.1)					
1042	Hexachlorobiphenyl	* + $													1.0 (0.2)					
1044	DDT	* + $													1.0 (0.1)					
1069	p-Nitrophenol	*													1.0 (0.2)					
1082	2,4-Dichloronaphthalene	*														1.0 (0.1)				1.0 (0.9)
	COMPOUNDS NOT ON THE SPECIFIC SEARCH LIST																			
26	1,1,2,2-Tetrachloroethane	$		5.0		3.0†			3.0†		7.0†	6.0†	6.0†		6.0†			4.0†	0.0†	
77	Phenanthrene	+	-1.0		2.0†		1.0†	0.0†		6.0	2.0†	2.0†		2.0†	3.0†		3.0†		1.0	
92	Naphthalene	+			1.0		4.0			6.0	6.0					1.0	1.0			
164	Pyrene	+			3.0					5.0	1.0†									
172	Ethylbenzene	$		4.0	5.0†	2.0†		0.0†					1.0†						1.0†	
173	p-Xylene	$		4.0	5.0†	2.0†		0.0†									1.0†			
306	1,2-Dichloroethane	$			4.6								4.0							
324	Toluene	$		3.0	4.0†	1.0†							4.0†			4.0†				
380	Anthracene	+					1.0		1.0	4.0										
511	m-Xylene	$			3.0							3.0	3.0				1.0			
523	Cumene	$			3.0				1.0	1.0										
528	o-Dichlorobenzene	+ $			2.0				1.0	3.0										
616	m-Dichlorobenzene	+ $							1.0			3.0								
620	2,3,4,6-Tetrachlorophenol	$								3.0										
621	2,4,5-Trichlorophenol	$								3.0										
649	o-Chlorophenol	$									3.0									
744	Acenaphthalene	+		2.0				0.0†			1.0†				1.0†		0.0†		0.0†	0.0†
750	o-Xylene	$			2.0								1.0							
753	Fluorene	+			1.0		1.0		1.0					2.0	2.0				2.0	
951	n-Propylbenzene	$			1.0															
1043	DDE	+ $												1.0	1.0					
	PHTHALIC ACID DIESTERS																			
3	Di-n-butyl phthalate	+ $	2.0		9.0	5.0†	7.0	5.0†	9.1			3.0†	3.6†	8.1	7.1	7.0	5.0†	8.1	6.0†	5.0†
8	Dioctyl phthalate	+ $			6.0						6.0			8.0	7.0			2.0		
41	Butyl butoxyethyl phthalate	$				7.0											2.0			
57	Butyl methyl phthalate	$							4.0	3.0			7.0	4.0	4.0	3.0	1.0	4.0		
69	Diethyl phthalate	+ $		1.0		3.0†							2.0†	5.0	6.0	3.0†		6.0		
81	Diisobutyl phthalate	$			5.0		4.0†		6.0			2.0	3.0†	5.1	6.0	3.0†		5.0		
82	Dicyclohexyl phthalate	$	3.0						2.6†							6.0		5.0†		5.0†

(continued)

TABLE 15. (Continued)

Seq. No.[a]	Compound	Special Interest List[b]	Relative Size[c] of GC Peak for Detection in the Indicated Concentrate[d]																	
			V1C	X1C	L2P	L2M	L2N	L2D	C3C	C1P	C1M	C1N	C2N	R1C	R2C	E1C	D2N	B2C	B1M	B1N
83	Bis(2-ethylhexyl) phthalate	+ $	2.6			2.0			2.0	6.0			1.0	6.0		2.0	3.0		5.0	
94	n-Butyl isobutyl phthalate	$			5.0		6.0				3.0				6.0	3.0		6.0		
97	Methyl ethyl phthalate	$			5.0						6.0									
158	Butyl benzyl phthalate	+ $							5.0	1.0	4.0		2.0					5.0		
197	Dimethyl phthalate	$			5.0				4.0			1.0		4.0	4.0	2.0		4.0	4.0	
332	Butyl butoxycarbonyl phthalate	$			4.0	4.0														
368	Dimethyl terephthalate	$				4.0			2.0											
396	t-Butyl methyl phthalate	$							4.0											
678	Di-n-propyl phthalate	$											3.0							
1091	Dihexyl phthalate	$	0.0																	

a) The sequence number corresponds to the entry in Table 10.

b) The three special interest lists are coded: *: list of 53 compounds for which the GC-MS was specifically searched (see Table 4). +: list of "Consent Decree Priority Pollutants." $: list of "Chemical Indicators of Industrial Pollution" Federal Interim Primary Drinking Water Regulations (February 9 1978).

c) See Section 5, Analytical Scheme/Quantification of Identified Compounds for an explanation of the Relative Size Parameter.

d) See Tables 8 and 2 for translation of the three digit concentrate code names. The symbol, †, designates a detection instance that may be attributable to the concentrate generation blank.

search compounds (not shown in Table 10) are shown in parentheses below the RS value entry in Table 15. Phthalates are listed separately in Table 12 to facilitate visualization of occurrence patterns for these high interest compounds.

The three samplings which reflected the highest levels of organic compounds in the sampled water (Pomona I, Lake Tahoe, and Orange County II at 370, 306 and 144 μg/l, respectively) also resulted in the detection of the highest number of search compounds at 16, 13 and 22 detections, respectively, as above. There are 117 detection instances shown for the 33 search compounds listed in Table 15; 10 of the 33 compounds account for 78 (67 percent) of those 117 detection instances; and 14 of the compounds were detected in only one concentrate. Table 15 also shows the specific search results for the Poplarville, V1C, DW concentrate since it functioned as the RO process blank. The detection of four compounds in concentrate V1C has resulted in the classification of 20 of the AWT concentrate detection instances as possibly attributable to the RO process blank, as indicated by the symbol, †. Since concentrate V1C does correspond to a sampling of finished DW instead of reagent water the possibility remains that these 4 search compound detections in V1C were present in that sampled water rather than introduced by the RO process. Thus, the 14 compounds designated as possibly due to the blank may, indeed, represent genuine detection instances. The search compounds for which some of the detection instances were at relatively high levels (10 ng/l or higher) were diphenyl amine, pentachlorophenol, 2,4,6-trichlorophenol, 2-chloroaniline, phenol, tricresyl phosphate and 2,4-D. In the section of Table 15 showing the detection instances for phthalates, those concentrates showing extremely high levels of dibutyl phthalate are L2P, L2N, C3C, R1C, R2C, E1C and B2C. In preceding discussions, the dibutyl phthalate detections in these concentrates were noted as probably artifacts. Since the source of the dibutyl phthalate contamination was probably an impure one, some of the other phthalate detections listed (expecially iso-butyl and mixed, monobutyl ones) are probably also artifacts.

Occurrence of Molecular Functional Groups in the Identified Compounds--

Associated with each identified compound entered in the computer-managed data base are a set of molecular functional group descriptors. Tabulations of the occurrences of the 25 functional groups in the AWT concentrate results is presented in Tables 16 and 17. Percentages which each of the 25 functional group classes represent of the total number of identified compounds are shown in Table 16. Display of the percentage of the total parameter in Table 16 was chosen to facilitate comparison of the relative distribution of the functional groups among the analyzed concentrates. Thus, Table 16 provides comparative information on the numbers but not the amounts of compounds with the various function groups. Total RS values for each functional group are shown in Table 17, and this parameter reflects the amounts of material for each functional group rather than the number of occurrences. Thus, these two tables are complimentary in the nature of the information provided. Note that the total number of identified compounds for each concentrate has been added to Table 16 to enable computation of the number of functional group occurrences from the percentages shown. Since these computer-printed tables (Tables 16 and 17) are generated from the data base before correction

TABLE 16. OCCURRENCE OF MOLECULAR FUNCTIONAL GROUP TYPES IN AWT CONCENTRATES, SHOWING THE NUMBER OF OCCURRENCES AS A PERCENTAGE OF THE TOTAL NUMBER OF IDENTIFIED COMPOUNDS

OCCURRENCE OF FUNCTIONAL GROUPS AMONG THE IDENTIFIED ORGANICS

PERCENT OF TOTAL

	V1C	X1C	L2P	L2M	L2N	L2D	C3C	G1P	C1M	C1N	C2N	R1C	R2C	E1C	D2N	B2C	B1M	B1N
1. UNSUBSTITUTED ALIPHATIC	3	8	1	2	11	3	5	1	2	3	2	3	2	0	4	0	4	1
2. HALOGENATED ALIPHATIC	0	4	2	2	1	2	2	1	2	4	2	1	2	4	4	3	3	3
3. SUBSTITUTED ALIPHATIC	51	54	19	47	31	34	23	27	35	30	44	40	41	38	43	48	48	45
4. UNSUSBSTITUTED ALICYCLIC	0	0	3	0	5	2	0	3	0	3	0	1	1	2	1	2	0	2
5. HALOGENATED ALICYCLIC	0	0	0	0	0	0	0	0	0	1	0	3	2	0	0	0	0	0
6. SUBSTITUTED ALICYCLIC	7	12	7	14	9	10	2	3	3	9	12	5	7	7	8	5	11	15
7. UNSUBSTITUED AROMATIC	10	8	55	6	28	17	37	43	19	19	7	9	14	7	14	6	11	4
8. HALOGENATED AROMATIC	7	0	2	2	4	7	9	6	5	9	3	14	8	13	6	10	4	4
9. SUBSTITUTED AROMATIC	27	12	15	29	29	34	36	24	31	25	29	31	24	47	30	38	21	14
10. UNSUBSTITUTED PNA	5	8	35	4	12	8	23	30	14	12	6	6	8	4	7	0	6	2
11. HALOGENATED PNA	2	0	0	0	0	0	1	0	0	1	0	2	2	0	0	1	0	1
12. SUBSTITUTED PNA	2	2	2	3	3	1	2	3	4	2	2	1	1	2	2	1	1	1
13. ALCOHOL GROUP	22	25	13	20	17	16	11	15	17	16	20	19	19	25	16	28	31	28
14. ALDEHYDE GROUP	2	2	1	2	1	1	0	1	2	2	2	1	2	2	1	1	1	1
15. AMIDE GROUP	0	0	0	0	1	1	1	1	3	2	4	3	0	0	1	1	1	2
16. AMINE GROUP	5	0	2	1	2	2	4	4	5	5	5	1	2	2	0	1	1	0
17. CARBOXYLIC ACID	25	25	7	29	26	43	14	9	27	23	33	28	29	33	45	45	29	36
18. ESTER GROUP	34	10	13	17	6	5	14	13	9	3	14	13	11	20	10	16	9	7
19. ETHER GROUP	3	10	6	16	11	16	9	8	14	17	12	10	9	11	10	7	15	16
20. HETEROATOM IN RING	7	12	3	4	7	7	2	5	14	12	12	7	6	4	3	3	9	8
21. KETONE	8	15	4	16	8	15	3	5	12	16	6	8	7	18	12	8	18	20
22. NITRO GROUP	2	2	1	6	1	4	1	1	1	1	1	2	4	5	3	2	3	4
23. PHTHALIC DI-ESTER	10	2	3	5	2	1	11	3	3	2	6	5	3	15	4	7	2	2
24. PHENOL GROUP	10	0	4	2	8	7	4	9	8	4	3	7	4	11	4	10	7	6
25. SULFUR ATOM	3	0	0	1	3	2	2	1	3	3	3	3	2	2	3	2	2	2
TOTAL NUMBER OF IDENTIFIED COMPOUNDS	50	52	260	133	157	178	114	158	153	95	120	125	255	55	113	124	141	126

* PERCENTAGE IS BASED ON THE TOTAL NUMBER OF IDENTIFIED COMPOUNDS RATHER THAN THE TOTAL NUMBER OF FUNCTIONAL GROUPS FORMED. THUS, THE SUM OF THE PERCENTAGES FOR A CONCENTRATE WILL TOTAL MORE THAN 100 PERCENT.

TABLE 17. OCCURRENCE OF MOLECULAR FUNCTIONAL GROUP TYPES IN AWT CONCENTRATES, SHOWING THE TOTAL GC PEAK SIZE FOR EACH GROUP ON BOTH GC COLUMNS

OCCURRENCE OF FUNCTIONAL GROUPS AMONG THE IDENTIFIED ORGANICS

COL. 1 TOTAL RS

		V1C	X1C	L2P	L2N	L2N	L2D	C3C	C1P	C1M	C1N	C2N	R1C	R2C	E1C	D2N	B2C	B1M	B1N
1.	UNSUBSTITUTED ALIPHATIC	0.0	-	5.2	2.2	5.3	8.3	6.1	0.0	4.0	4.5	5.6	4.0	5.2	-	4.1	-	5.3	0.0
2.	HALOGENATED ALIPHATIC	-	2.2	5.2	3.6	0.0	7.0	0.0	0.0	6.3	6.0	5.0	3.0	0.0	3.1	2.2	4.9	3.3	3.4
3.	SUBSTITUTED ALIPHATIC	3.4	6.0	7.7	10.1	8.5	9.4	10.1	8.4	7.8	7.9	7.9	8.4	8.9	6.7	6.8	7.6	7.3	7.1
4.	UNSUSBSTITUTED ALICYCLIC	-	-	5.9	-	4.8	6.1	-	6.3	-	4.5	-	4.4	5.2	0.0	1.0	5.0	-	2.0
5.	HALOGENATED ALICYCLIC	-	-	-	-	-	-	-	-	-	0.0	-	0.0	1.0	-	-	-	-	-
6.	SUBSTITUTED ALICYCLIC	0.4	4.5	6.1	6.9	5.4	8.1	1.0	6.3	5.8	6.1	6.2	4.0	5.9	3.5	4.3	4.9	6.0	5.6
7.	UNSUBSTITUED AROMATIC	0.2	4.8	7.4	2.7	5.5	8.6	4.7	7.5	6.2	5.5	5.1	4.6	4.5	4.1	3.9	5.2	6.2	2.8
8.	HALOGENATED AROMATIC	0.5	-	3.8	7.0	4.0	8.5	5.3	5.2	6.4	7.4	7.0	5.1	4.7	4.3	4.5	4.9	4.8	3.7
9.	SUBSTITUTED AROMATIC	2.6	4.6	9.2	7.9	7.5	9.9	9.1	8.4	7.7	7.8	7.6	8.5	8.0	7.2	6.2	7.9	7.0	5.9
10.	UNSUBSTITUTED PNA	-1.0	4.8	7.1	2.2	4.5	2.3	4.4	7.2	6.2	4.4	2.9	3.0	3.9	4.0	3.1	-	4.2	0.6
11.	HALOGENATED PNA	-1.0	-	-	-	-	-	1.0	-	-	1.0	-	0.0	2.0	-	-	0.0	-	1.0
12.	SUBSTITUTED PNA	-1.0	4.0	6.1	5.7	3.1	3.0	1.6	1.0	5.2	5.3	3.0	0.0	2.2	3.0	0.6	0.0	2.0	1.0
13.	ALCOHOL GROUP	1.9	5.0	7.3	7.7	8.4	8.1	9.2	7.6	7.3	6.8	6.6	7.1	8.1	6.7	6.2	7.2	7.2	6.6
14.	ALDEHYDE GROUP	-1.0	0.0	3.2	3.1	1.0	0.0	-	0.0	5.4	5.2	4.1	0.0	2.2	3.0	0.0	3.0	2.6	1.0
15.	AMIDE GROUP	-	-	1.0	-	2.0	1.0	6.0	6.0	5.3	4.2	4.0	4.9	1.0	-	0.0	3.0	0.0	2.2
16.	AMINE GROUP	-0.4	-	5.4	1.6	3.4	3.3	3.2	8.1	5.3	4.6	4.1	2.0	4.2	1.0	-	0.0	4.2	-
17.	CARBOXYLIC ACID	2.7	5.3	6.4	7.4	6.9	10.4	5.7	5.5	7.4	8.0	7.9	8.0	8.5	5.5	6.7	7.4	7.3	6.9
18.	ESTER GROUP	3.3	4.9	9.2	6.6	7.0	7.6	9.1	8.1	6.9	4.3	6.5	8.6	8.2	7.1	5.7	7.7	6.3	5.5
19.	ETHER GROUP	2.2	4.3	7.2	8.2	8.4	8.8	10.1	6.1	7.6	7.5	7.3	6.9	7.8	6.3	5.2	6.5	6.7	6.4
20.	HETEROATOM IN RING	2.3	4.3	5.0	3.6	5.7	7.3	4.1	6.3	7.1	6.4	6.1	5.2	5.6	0.0	2.7	6.1	4.9	4.6
21.	KETONE	2.1	3.8	5.8	6.8	5.3	7.9	3.2	5.0	7.0	6.7	4.5	5.2	5.5	5.0	4.9	5.7	6.3	5.6
22.	NITRO GROUP	1.0	5.0	3.6	6.6	5.6	7.4	1.0	5.0	5.6	5.2	5.0	4.4	5.0	2.7	4.1	4.3	5.3	4.4
23.	PHTHALIC DI-ESTER	2.2	0.0	9.1	5.2	7.0	4.0	9.1	0.0	6.0	3.1	2.6	8.2	7.4	7.0	5.0	7.5	6.1	5.0
24.	PHENOL GROUP	1.4	-	6.4	4.1	5.3	7.1	5.1	7.1	6.3	5.9	5.1	5.4	5.4	3.8	3.5	5.4	6.1	4.6
25.	SULFUR ATOM	1.0	-	3.0	3.0	5.1	7.0	6.1	6.2	6.0	5.8	5.6	4.6	3.5	3.0	2.7	4.3	3.2	3.0

for the blank, the total numbers of identified compounds shown in Table 16 are also uncorrected for the blank.

For 13 of the functional group classifications of Table 16, the percent occurrence values are either low or there is not sufficient variation in them among the AWT concentrates to require any discussion. These 13 classifications are: unsubstituted aliphatic, halogenated aliphatic, unsubstituted alicyclic, halogenated alicychic, halogenated PNA, substituted PNA, aldehyde group, ester group, amide group, amine group, nitro group, phenol group, and sulfur atom. Observations concerning the remaining functional group types are the following:

- Comparing the molecular nucleus classifications, substituted aromatic, substituted alicyclic and substituted aliphatic, shows that, for the non-halogenated species, non-aromatic molecular nucleii were more numerous than aromatic molecular nucleii in all concentrates except E1C and C3C. Large numbers of phthalates, which are classified as containing an aromatic nucleus, partially explain the exceptions for E1C and C3C (see the discussion, below, on the phthalate functional group).

- The high values shown for unsubstituted aromatic and unsubstituted PNA for concentrates L2P, C3C and C1P are related to the high numbers of alkyl benzenes and naphthalenes that were identified in the aromatic fractions of these three concentrates. In the assignment of functional groups, molecules with only alkyl (or alkenyl) substitution are classified as unsubstituted, and aromatic ring systems larger than benzene are classified as a PNA molecular nucleus.

- Concentrates R1C and E1C have marginally higher occurrence percentages for the halogenated molecular nucleus, and the Lake Tahoe and Blue Plains I concentrate sets are somewhat below average for this value.

- Little variation was observed for the relative numbers of identified alcohols except for the Blue Plains I and II concentrates (B2C, B1M and B1N) which are significantly above the average. The higher proportion of alcohols for these three concentrates can partially be attributed to a greater variety of poly glycols among the identified compounds.

- The carboxylic acid substituent group was the predominant one found for all concentrates except the two prepared by pentane extraction of the RO brine (L2P and C1P). This result was not surprising based on the polarities of the extraction solvent. In two of the three cases for which both the unbuffered methylene chloride and the acidified methylene chloride extracts were analyzed (L2M/L2N, C1M/C1N and B1M/B1N) a slightly higher proportion of carboxylic acids were identified in the concentrate from the unbuffered extract (L2M and C1M).

This result is in contradiction to the expected one, and is addressed in a subsequent section of this volume.

- Slightly elevated detection frequencies for the heteroatom in ring functionality in concentrates C1M, C1N and C2N reflect detection of the following materials: barbiturates (four species in C1M, one in C1N), saccharin (C2N), ethosuximide (C1M), pentachloropyridine (C1N), caffeine (C1N), nicotine (C1M), quinolines (C2N), isoquinolines (C2N), pyridines (C1M and C2N), piperidines (C2N), pyrimidines (C2N), and pyrrolidines (C2N).

- The percentages of compounds with the ketone goup were slightly elevated for about half the concentrates (L2M, L2D, C1M, C1N, E1C, B1M, and B1N).

- The two concentrates (C3C and E1C) in which the artifact level of dibutyl phthalate was the highest show distinctly higher percentages of the identified compounds were phthalates (i.e., in addition to dibutyl phthalate). This results from two effects: 1. The dibutyl phthalate concentration was so high that the accompanying impurity levels of seldom encountered phthalates were at easily detectable levels, and 2. The phthalate chromatographic overloading resulted in less effective identification of other compounds, reducing the total number of identifications.

Since RS values span a logarithmic scale, the total RS value shown in Table 17 is not an arithmetic sum of the individual RS values since such a sum of logarithmic scale values would be mathematically related to the product of individual GC peak heights rather than the sum of them. For example, 10 GC-MS peaks, each with an RS value of 1.0 would give a total RS value of 3.0, and two peaks with RS values 2 and 8 would yield a total RS value of 8.0009. The mathematical basis of the GC-MS peak RS parameter is detailed in Section 5, Analytical Scheme. For the purposes of interpreting Table 17, it suffices that an arithmetic difference of 1.0 between two total RS values in the table under comparison corresponds to a factor of one-half of an order of magnitude (3.16) change in the amount of material represented; a difference of 2.0 in total RS values corresponds to a factor of one order of magnitude (10.0), and so forth.

The AWT concentrate functional group results, expressed as the total RS value for each classification catagory, are shown in Table 17. Some of the characteristics of the AWT concentrates which the values in Table 17 reflect are discussed below.

The predominant type of molecular nucleus (catagories 1-12, Table 17) were, as expected, the substituted aliphatic and substituted aromatic catagories with these taking the highest and second highest total RS values for each concentrate. Although 10 of the 16 concentrates have the substituted aliphatic catagory with highest total RS value (an eleventh, C1P, had equal total RS values for the two nucleus types) this predominance probably does not reflect the organic material present in the original water since 8 of those 10 concentrates are the separate methylene chloride extracts of RO brine (C2N, D2N, L2M/L2N, C1M/C1N and B1M/B1N) and the prior extraction of RO brine with pentane had removed a significant portion of the aromatic material. For 3 of the 4 composited concentrates (B2C, E1C and R1C), the substituted aromatic nucleus had the highest total RS value. For the 2 pentane extract concentrates, L2P had the substituted aromatic nucleus with the highest total RS and C1P had the substituted aliphatic and aromatic nucleii with equal total RS values. On the other hand, high levels of dibutyl phthalate (classified as containing the substituted aromatic molecular nucleus) exerted a controlling influence on concentrates R1C, E1C, B2C and L2P. The high levels of poly glycols (classified as the substituted aliphatic nucleus) exerted a similar controlling effect for concentrates L2M, L2N, C1M, C2N, R2C, D2N, B1M and B1N. If both the butyl phthalate and poly glycols were present as artifacts, no conclusion concerning the predominant type of molecular nucleus in the original water can be made. The halogenated aromatic nucleus was ranked with the third highest total RS value in 7 cases (L2M, C1M, C1N, C2N, R1C, E1C and D2N) and fourth highest in 3 cases (L2D, C3C and B1N).

In the 13 catagories of substituent groups (13 through 25 in Table 17), the presence of very high levels of butyl phthalate and poly glycols exerts an obscuring effect similar to that noted above for the type of molecular nucleus. Butyl phthalate contributed to the total RS values for the ester and phthalate groups, and these two groups have the highest two RS value rankings for concentrates L2P, R1C, E1C and B2C which contained dibutyl phthalate at high, artifact levels. Poly glycol compounds were classified as containing the ether and alcohol functional group, and these two groups were among the 5 highest total RS values for all concentrates except C1P. Eight concentrates (L2M, L2N, C2D, C1M, C1N, C2N, B1M and B1N) had the alcohol and ether group as two of the 3 highest total RS value substituent groups, and, in all but one case (L2N), the carboxylic acid substituent was the other group of the three. The carboxylic acid group was among the 5 with highest RS values for all concentrates except C1P and C3C. Ketones had the fourth highest total RS value for 5 concentrates (L2M, L2D, C1N, B1M and B1N) and the fifth highest in one case (C1M). The heteroatom in ring group had the fourth highest total RS value in concentrate C1M and the fifth highest value in concentrates C1P, C1N and C2N. The compounds which contributed significantly to the heteroatom in ring total RS values for these four concentrates were (in decreasing order of RS values): benzthiazole (all four concentrates), barbiturates (C1M and C1N), saccharin (C1N, C2N), dimethyldihydroacridine (C1P), methoxbenzisothiazole (C1M), benzisothiazolone (C1M), a reduced keto-azepine (C1N, quinolines and isoquinolines (C2N and C1P), ethosuximide (C1M), caffeine (C1N), nicotine (C1M), dimethylindole (C1M), a reduced pyridine (C2N), and N-propyl succinamide (C1P).

The substituent groups which were among the three for each of the 16 concentrates with the lowest total RS values were distributed as follows:

Functional Group	Number of Concentrates for which the Indicated Functional Group was Found Among the Three Lowest Total RS Value
amide	14
aldehyde	13
amine	11
sulfur atom	5
phthalic diester	3
nitro	2
ketone	2
ether	1
ester	1

Four additional functional group tables for the AWT concentrates are presented in Volume 2. Three of these tables show the number of occurrences, the total RS parameter for SP1000 GC-MS analysis and the total RS parameter for SP2100 GC-MS analysis using a format identical to Tables 16 and 17. The fourth table shows all five parameters for each concentrate (i.e., those of Table 16 and Table 17 plus the other three cited above) in close proximity groupings for each concentrate to facilitate simultaneous comparison of all five parameters between concentrates.

The Effect of Concentrate Production Methodology on the Compound Identification Results--

The 16 AWT concentrates analyzed were produced using RO preconcentration as the first step (with cellulose acetate and nylon units processing the water in series) followed by liquid-liquid solvent extraction of the two RO brines produced for each concentrate (see Section 4). Four of the concentrates were a composite of all six solvent extracts of RO brine (C3C, R1C, E1C and B2C) and the other 12 concentrates were individual extracts of RO brine. Based on the compound identification results, some conclusions can be made regarding the types of compounds that can be recovered in the separate RO brine extracts.

Concentrate L2D was the only separate RO brine extract analyzed that was produced from the nylon unit RO brine. If the cellulose acetate RO unit had retained all of the organic materials in the sampled water, concentrate L2D should have been devoid of organic compounds. The listings of Tables 7, 9 and 17 show that just the opposite was the result, and concentrate L2D contained comparable amounts of material (relative to L2M and L2N) amenable to GC-MS analysis. Analysis of additional concentrates enabling comparison of cellulose acetate and nylon RO extract pairs would be required to determine whether the anomalous L2D results were caused by some malfunction of the cellulose acetate RO module or whether they correctly reflect a very poor performance capability for the cellulose acetate RO unit. Obviously, correctness the latter possibility would have a serious impact on this work.

As expected, the first RO brine extract, using pentane, contained more apolar materials (especially aromatic hydrocarbons) and less strongly polar material, (especially carboxylic acids) compared to the two methylene chloride extracts. The pentane concentrates (L2P and C1P), nevertheless, contained surprisingly high levels of many moderate polarity neutrals. Comparison of the total RS values for concentrates L2P and C1P in Table 17 with other methylene chloride extract concentrates adequately illustrates this point. These surprisingly high recoveries of polar species may have been due to the strong salting out effect of the RO brine ionic strength combined with the mass action effect of the high levels of organic material present in the aqueous phase. Addition of an ethanol or methanol back extraction of the partially concentrated pentane extract with re-combination of the alcohol phase and the RO brine would have produced a pentane concentrate containing lower levels of polar species.

The compound identification results indicate that the RO brine extraction procedure of unbuffered methylene chloride extraction failed to produce the expected result of recovery of acidic materials preferentially into the latter extract. The concentrate pair B1M/B1N illustrates this failure clearly, and comparison of the other pairs, L2M/L2N and C1M/C1N, give essentially the same results. The GC-MS chromatograms of the acid, medium polarity and high polarity fractions of B1M and B1N were so similar that they could almost be superimposed in most regions. Not surprisingly, there was a high degree of correspondence between the sets of compound identification results for B1M and B1N. The principal differences were that the pH 2 extract, B1N, contained more or higher concentrations of higher strength or more polar acids. Surprisingly, many acids were recovered better or exclusively in the unbuffered extract, B1M (for example, clofibric acid, 2-ethylhexanoic acid and ethosuximide). One explanation for these results would be that the unbuffered pH was more acidic than the pH 5.5 reported for cellulose acetate RO processing (pH 10 was used for the nylon RO unit). An uncontrolled pH for the first methylene chloride extraction would account for the variability of acid species enhancement for the pH 2 extract (compare total RS values in Table 17 for the carboxylic acid group and the identified compounds in Table 10 for concentrate pairs L2M/L2N, C1M/C1N and B1M/B1N).

The near exclusion of basic species from the compound identification results probably was due to a failure of the concentrate production system to recover these species. Most of the compounds which contributed to the amine group total RS values in Table 17 were of very low base strength (for example, diphenylamine was found with RS value 8.1 in concentrate C1P). While the protonated bases would probably have been retained efficiently by the cellulose acetate RO unit (operated at pH 5.5), these species would have been very poorly recovered by extraction from the cellulose acetate RO brine since no extractions were performed at basic pH. Bases which permeated the cellulose acetate membrane and were retained by the nylon membrane (operated at pH 10) could have been recovered by the first and second extractions (pentane and unbuffered methylene chloride), and these circumstances may account for the small number of basic species that were observed. An alternative recovery mechanism would be an ion pair extraction mechanism during the unbuffered cellulose acetate methylene chloride extraction.

One unfortunate effect of the concentrate production method had on the analysis results was the apparant contamination of certain concentrates (Pomona I, Pomona III, Escondido, Orange County I and Blue Plains II) with very high levels of dibutyl phthalate. The presence of similarly high levels of poly glycol materials in some of the concentrates did not correlate with the phthalate artifact, but the levels of these poly glycol materials varied over such an extremely wide range that they must also be considered as possible artifacts. However, since use of these materials in soaps, cosmetics and ointments is common, they are expected at relatively high levels in sewage, and the variability of their levels in the concentrates might be explainable in terms of variations in AWT plant performance. Since these poly glycols are hydrophilic, they might be among the first of the organic materials to break through a GAC contactor as the adsorption capacity is consumed.

Effect of the Raw Water Source on the Analysis Results—

Apparantly, the effectiveness of the AWT plant exerted a greater controlling influence on the organic material present in the AWT concentrates than did the nature of the plant influent water since there are no obvious correlations between the source water (described in Table 2) and the compound identification results. In addition, no conclusion can be made concerning the effect the time of year of sampling had on the nature of the concentrate since all of the multiple samplings at significantly different times of year at a given site (Pomona and Blue Plains) corresponded to a change in the AWT plant design. The only noteworthy observation in this regard was that a variety of oxygenated diterpene compounds were found in the Lake Tahoe concentrates (especially L2P), but these compounds are probably more related to precipitation run off than wastewater discharges. With regard to the AWT plant effectiveness, the analysis results indicate that the Escondido AWT plant, which was based on RO treatment rather than GAC contactor treatment as for all the other plants (see Table 2), produced product water containing substantially less organic material than the other plants. Comparison of the results shown in Table 8 for E1C with those of the other AWT concentrates adequately documents this conclusion.

COMPARISON OF DW AND AWT CONCENTRATE COMPOUND IDENTIFICATION RESULTS

In Section 6, Overview, some conclusions regarding the comparison of DW and AWT concentrates were reached on the basis of the information presented in Tables 7 and 8. Those conclusions are briefly summarized below:

- Of the organic material recovered in the analyzed fractions, most was contained in the acid and high polarity fractions (averages of 94 and 97 percent for DW and AWT concentrates, respectively).

- The percentage of the original concentrate material which could be recovered into the analyzed fractions was about the same for DW and AWT concentrates, averaging 52 percent for both.

- The relative amounts of the material (versus the original concentrate) recovered in the acid and high polarity fractions for DW and AWT concentrates was substantially different, with DW concentrates averaging 32 and 18 percent in the acid and high polarity fractions, respectively, and AWT concentrates averaging 16 and 33 percent for the acid and high polarity fractions, respectively.

- On the basis of the concentration in the original water that the concentrates represented, the DW concentrates were consistantly and, in some cases, higher than the AWT concentrates.

Comparison of the tables listing the total RS values for 25 functional groups for the DW and AWT concentrates (Tables 14 and 17, respectively) shows that carboxylic acids and phenols represented higher concentrations of compounds in DW concentrates than these functional groups did in AWT concentrates. The average values are 8.1 versus 7.0 for carboxylic acids and 5.6 versus 5.02 for phenols for the 7 composited solvent extract type DW concentrates versus the 5 composited solvent extract type AWT concentrates. Thus, these comparisons agree with the relatively higher amount of material in the DW concentrate acid fraction compared to the AWT concentrate acid fraction.

A predominant feature of the AWT concentrates was a variable but usually very high level of poly glycols. This class of compounds was recovered in the high polarity fraction, accounting for the higher portion of the AWT concentrates, relative to the DW concentrates, recovered in that fraction. While poly glycol species were usually represented in the DW concentrates, none of them approached the very high levels observed for the AWT concentrates. The total RS values for the ether functional group in Tables 14 and 17 reflect the higher amounts of these poly glycols in the AWT concentrates. The average total RS values for the ether group were 7.5 and 7.2 for the AWT and DW concentrates, respectively, as above. The ether group is less sensitive for demonstrating the presence of poly glycols than is the carboxylic acid group for the amount of material in the acid fraction since other compounds commonly encountered at high levels (for example, clofibric acid) also contain the ether linkage. The significance of the ether group total RS values cited above is reinforced by similarly comparing the ketone functional group which is also encountered predominantly in the high polarity fraction. The average total RS values for the ketone group are 4.9 and 6.9 for the AWT and DW concentrates, respectively. Note also that the poly glycol compounds that are identified specifically enough for entry into the data base are lower molecular weight oligomers which represent only 5 to 10 percent of the GC-MS peak areas of the higher molecular weight poly glycol oligomers. Although these higher molecular weight oligomers were observed in the GC-MS data, they were not specifically identified, on a molecular basis and, thus, did not contribute to the ether group total RS values in Tables 14 and 17.

The compound identification results for both the DW and AWT concentrates are shown is a single, integrated listing in Table 11 (note, some of the concentrates have been omitted from Table 11 due to space limitations; see the relevant discussion in Section 6, Overview). Table 11 facilitates the comparison of DW and AWT compound identification results on the basis of frequency and levels of detection for each compound. Most of the compounds listed in Table 11 have relatively isolated detection instances which cannot reasonably be used to infer a pattern of occurrence in the sampled water. The compounds which do have a sufficient number of detection instances in Table 11 to justify classification as predominantly occurring in either DW or AWT water or both have been assembled in Table 18 to further facilitate comparison of the types of compounds identified in DW and AWT concentrates. The compounds shown in Table 18 have been listed in the order that they appear in Table 11 and arranged on the page to spatially approximate the position of occurrence in Table 11. In addition, the glycol ethers and poly glycol compounds have been omitted from Table 18 since there are so many of these species and careful attention was not taken to maintain consistency in their identification assignments (all of which were intentionally left tentative). Some of the conclusions which can be drawn from Table 18 are the following:

- DW concentrates show a greater tendency for recurring detections of compounds with 39 compounds indicated as identified principally in DW concentrates and only 12 compounds indicated as identified principally in AWT concentrates.
- A higher portion of recurring identifications in AWT concentrates are for materials related to domestic sewage. Examples are drug related compounds (phenobarbital, clofibric acid, salicylic acid and ethosuximide) and food related materials (saccharin, benzoic acid, caffeine and BHT). Nicotine is the only compound qualifying for this class of substances among the 39 compounds shown for DW concentrates.
- Bromohaloforms were detected nearly exclusively in DW concentrates.
- Non-aromatic halogen containing compounds (12 species) are found in Table 18 only as predominantly DW identification occurrences.
- There was a somewhat greater tendency for aromatic compounds to be found in AWT concentrates. The relative amounts of compounds with an aromatic moiety were 67, 73 and 28 percent for the AWT only, both AWT and DW and DW only groupings in Table 18. This result is also reflected by comparing the listings in Tables 16 and 13 of the percentage of identified compounds in AWT and DW concentrates which contained the substituted or unsubstituted aromatic nucleus. The averages for the 5 AWT and 7 DW concentrates (as above) are 50 and 34 percent, respectively.

TABLE 18. DISTRIBUTION OF COMPOUND IDENTIFICATION INSTANCES FOR DW AND AWT CONCENTRATES

Sequence Number*	Compounds Identified Principally in DW Concentrates	Sequence Number*	Compounds Identified in Both DW and AWT Concentrates	Sequence Number*	Compounds Identified Principally in AWT Concentrates
34	cyclohexanone	1	clofibric acid		
42	butyric acid	14	methylethylmaleic acid		
46	dichloroacetone	35	benzoic acid	8	tris-2-chloroethyl phosphate
56	bromodichloromethane				
57	bromoform				
72	phenylacetic acid	70	salicylic acid		
80	2-pentanol				
81	3-penten-2-ol	95	ethosuximide		
129	acetophenone			107	phenobarbital
135	isophorone				
148	valeric acid	133	m-toluic acid		
149	trichloroacetic acid	134	p-toluic acid		
150	triethylphosphate				
163	dicamba (3,6-dichloro-2-methoxylbenzoic acid)				
142	dibromochloromethane				
197	o-dichlorobenzene				
211	trichloropropenoic acid	193	cyclohexenone		
240	2,3-dimethylbenzoic acid	239	p-chlorophenol		
		243	2,4-D .		
		250	o-toluic acid		
		254	2,5-dimethylbenzoic acid		
320	2,4,5-T			258	2-chloroaniline
332	veratric acid	331	2,5-hexanedione	260	saccharin
343	2,2,6-trimethyl-1,4-cyclohexanedione			297	2,5-dimethylphenylbutanoic acid
345	isohexanoic acid				
363	anisic acid			341	3,5-dimethylbenzoic acid
364	tetrahydrotrimethylbenzofuranone				
365	1,3-dichloro-2-methylbutanoic acid				
384	diethylformamide				
454	2,3-dichloroaniline				
472	2-methyl-2-pentanol	419	5-methylhexanoic acid		
494	dalapon(2,2-dichloropropanoic acid)	444	dimethylformamide	455	dimethyl phthalate
499	4,4-dichlorobutenoic acid	451	p-dichlorobenzene		
		456	phenylacetonitrile		
528	3-methyl-2-cyclohexen-1-one	464	1,2,4-trichlorobenzene		
		507	caffeine		
		523	p-chlorobenzoic acid		
		535	2,4-dichlorophenol		
		538	2,2-dimethylbutyric acid	531	m-chlorobenzoic acid
617	1,1,3-trichloropropene			561	dimethyl sulfone
689	2,2,6-trimethylcyclohexanone				
690	2,3-dimethylbutyric acid				
752	3-methylcyclopentenone				
786	3-hydroxy-3-methyl-2-butanone	785	diphenylamine		
837	nicotine	845	2,6-dimethylpyridine		
		848	2,4,6-trimethylpyridine		
		860	BHT		
		872	pseudocumene		
1092	1,1,2-trichloropropene	1031	1,6-dimethyl-4-isopropylnaphthalene	886	2,6-dimethylheptanoic acid
		1032	1,2,3-trimethylbenzene		
1350	1,1,2,3,3-pentachloropropene	1368	2,3,6-trimethylnaphthalene	1160	fluorene
				1215	2-methylstyrene

* The sequence number corresponds to each compound location in Table 11.

TABLE 9. COMBINED LISTING OF IDENTIFIED COMPOUNDS FOUND IN DW CONCENTRATES

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COMBINED CONCENTRATE REPORT(PART I.A)

RELATIVE SIZE

	COMMON NAME	CAS NO.	*	VIC	VIX	T2B	T1C	T1X	T1Y	T4C	T4X	M2C	N2C	P2C	P2K	O2C	O2X	S2C	S2X	X1C	X1X
1	%+$DI-N-BUTYLPHTHALATE	84742		2.0	1.0	3.1	5.0		5.0		0.6*	0.7	0.3	0.1		4.0*		2.5*	1.2*		1.4
2	%+NAPHTHALENE	91203	a		5.1	1.0		5.0*		0.6	3.6*				7.0*	4.9	7.9*	2.2			2.2
3	2-ETHYL-1,1-BIPHENYL	1812517	A		6.0						3.6*			1.0	7.0*	0.3	4.9*				3.2
4	%PALMITIC ACID	57103				3.0	7.0			4.6*	3.6*	7.6	5.7*	5.0*	1.0*	4.9*	1.9*	5.2	1.2*	5.0	
5	%1-BUTANOL	71363						3.0				4.6	7.3		2.0				2.5		
6	2-HYDROXY-2-METHYLPROPANOIC ACID	594616							7.0			1.6									
7	2-ETHYL-3-METHYLMALEIC ACID	41654095					7.0	5.0		5.6	4.6	5.6	6.7	4.0		6.9	4.9	4.2	4.2		
8	1-(1-METHYLPROPOXY)-2-PROPANOL	53907952					7.0									0.9					
9	%METHYL BENZOATE	93583				7.0			5.0*												
10	%CYCLOHEXANOL	108930				5.0	5.3*	3.0		3.6*		6.9	5.0	5.9		5.0*		5.3		4.2	
11	%MONOBUTYL PHTHALATE	131704				1.0							6.7	6.0						2.0	
12	1,2 5,6-BIS-O-ISOPROPYLIDENE-BETA-D-TALO	23262795												6.0		5.9				4.2	
13	1,2 4,5-DI-O-ISOPROPYLIDENE-ALPHA-D-FRUC	20880937												6.0							
14	2,3-DIMETHYLMALEIC ACID	488211					5.0	4.0		5.6	4.6	5.6	6.7	5.0		5.9	4.9	4.2			
15	PHTHALIC ANHYDRIDE	85449											6.7								
16	%CYCLOHEXANONE	108941					5.0			2.6		6.7	5.7	5.0		3.9		4.2	1.2		
17	%BENZOIC ACID	65850		0.0	4.0	5.0	5.0	6.0	6.0	4.6	3.6	6.6	5.7	5.0	4.0	4.9	5.9	4.2	5.2	1.0	4.2
18	%MYRISTIC ACID	544638		1.0		3.0	6.0			3.6*		6.6	4.7			4.1	1.9*	5.2		4.0	3.2
19	PENTADECANOIC ACID	1002842		1.0		1.0	4.0*			2.6*		6.6	3.7*					3.2*		2.0	
20	%$DI-ISOBUTYLPHTHALATE	84695		0.0	1.0		5.0					6.6	6.0	3.0							
21	TRANS-2-METHYLCYCLOPENTANOL	25144041				2.0		4.0				6.6		5.4					3.2		
22	2-METHYLBUTYRIC ACID	116530							3.0	3.6	3.6	6.6	3.7	4.0	2.0	3.9	4.9	4.2	2.2		
23	2,2,4,4-TETRAMETHYL PENTANOIC ACID	3302123							3.0	2.6		6.6	3.7	3.0							
24	%BUTYRIC ACID	107926									4.6	6.6	2.7	2.0			2.9		3.2		
25	MARGARIC ACID	586127										6.6	2.7*					3.2*		3.0	
26	1,2-PROPYLENE GLYCOL, DIMETHYL ETHER	7778850										6.6									
27	2-HEPTENE	592778										6.6									
28	1,1-DICHLOROACETONE	513882										6.6	5.7	4.0							
29	3-ETHYL-4-METHYL-2,5-FURANDIONE	3552338										6.6	5.7			5.9		2.2			
30	2-HYDROXY-3-METHYL-2-CYCLOPENTEN-1-ONE	80717					4.0		5.0									6.2			
31	4-(HEXYLOXY)-1-BUTANOL	4541133												2.0		4.9		6.2			
32	6-BROMO-2-HEXANONE	10226296					4.1		6.1			4.6									
33	%BROMODICHLOROMETHANE	75274					1.0		6.1			2.6	1.7	0.0							
34	%BROMOFORM	75252					2.0		6.0	0.6		4.6	3.7								
35	4-METHYL-2-PENTANOL	108112			3.0	5.6		6.0	6.0*					5.0	4.0*		4.9*			1.0	
36	%*+$2,4,6-TRICHLOROPHENOL	88062		-2.0					6.0	3.6		0.6		4.0	-0.2			2.2			
37	%+$DIETHYL PHTHALATE	84662		0.0		2.0	3.0	3.0	6.0	1.6*	3.6	4.6	4.7			3.9			1.2*	1.0	
38	2,4,6-TRIBROMOPHENOL	2001							6.0												
39	AMYLENE DICHLORIDE	587459							6.0	2.6*		4.6	4.7	2.0*		2.9*		3.2	4.2	2.0	
40	%9,10-ANTHRACENEDIONE	84651							6.0												
41	7,7-DIMETHYL-2-OXOBICYCLO[2.2.1]HEPTANE-	3144169							6.0												
42	3-METHOXY-3-METHYL-2-BUTANONE	36687986							6.0			3.6	5.7					4.2			
43	4-HEXEN-3-ONE	2497214							6.0			3.6									
44	%TRICHLOROPROPANE	96184					6.0														
45	1-METHOXY-2-PROPANOL	107982				5.0	6.0	6.0						4.0	2.1	5.9	4.9		4.2		

* SEE LAST PAGE OF TABLE

(Continued)

TABLE 9. (Continued)

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COMBINED CONCENTRATE REPORT(PART I.A)

RELATIVE SIZE

	COMMON NAME	CAS NO.	*	V1C	V1X	T2B	T1C	T1X	T1Y	T4C	T4K	M2C	H2C	P2C	P2X	O2C	O2X	S2C	S2X	X1C	X1X
46	3-HEXANOL	623370						6.0				5.6	4.7	2.8	2.8		2.9	1.2			
47	XSALICYLIC ACID	69727			1.0	1.0	6.0	3.0	4.0	3.6	4.6	3.6	3.7	4.8	3.8	3.9	3.9		3.2		
48	XCAPRYLIC ACID	124072				1.0	6.0		3.0	3.6	1.6		5.7	4.8	3.8	3.9	1.9	3.2	3.2		
49	XPHENYLACETIC ACID	103822					6.0	4.8	3.0	3.6	3.6	4.6	4.7	5.8	4.8	4.9	4.9	2.2	3.2		
50	~~2,3-DIMETHYLMALEIC ACID~~ SEE NO. 14	~~400211~~					~~6.0~~			~~5.6~~	~~4.6~~					~~5.0~~					
51	XPELARGONIC ACID	112050					6.0						3.7	3.8		3.9		3.2	2.2		
52	XSTEARIC ACID	57114					6.0*			3.6*			3.7*			4.9*		5.2*		5.0	
53	1,3,5-TRIMETHYLCYANURIC ACID	827167					6.0		5.0	3.6			4.7								
54	1-METHYLBUTYLALCOHOL	6032297				3.0	3.6					5.7	6.0	4.9		4.8		4.5			
55	3-PENTEN-2-OL	1569502							4.0	3.2*		5.6	6.8	5.8		4.9				3.0	
56	2-METHYL-3-HEXANOL	617296													1.8*				-0.8*	6.0*	
57	2-ETHYLBUTANAL	97961																		6.0	
58	X4'-ETHYLACETOPHENONE	937304	A		4.0				4.0*		2.6*				5.9*		4.5*		1.2*		
59	DEHYDROABIETIC ACID	9155704		1.0	0.0	2.0				3.6*			2.7*			5.9		2.2*		1.0	1.2
60	3,4-DIETHYLBIPHENYL	61141660	A		5.3								1.7				5.9*				4.2
61	1-METHYL INDENE	767599	A		3.0						2.6*		0.7	8.8		5.9	1.9*				
62	XBTOLUENE	108883				5.0					3.6			4.8			5.9		2.2	3.0	
63	ISOVALERIC ACID	503742					4.0		4.0	2.6	4.6	3.6	3.7	4.8	4.8	4.9	5.9		4.2		
64	2,4-DIMETHYLBENZOIC ACID	611018							3.0	2.6			1.7	3.8		2.9	5.9	4.2	2.2		
65	3-PENTEN-2-ONE	625332														5.9		2.2		1.0	
66	HEXAHYDROTOLUENE	108872														5.9					
67	XACETOPHENONE	98862			3.0	1.6	2.0		5.1*		3.6*	4.6	3.7	4.9	5.9*	2.9	5.0*	2.2	1.3		
68	6-METHYL-5-HEPTEN-2-ONE	110930					3.1							3.8	5.9	2.9		2.2			
69	2-ETHYL-1-HEXANOL	104767		-1.0			4.0	5.0		4.2	4.6				5.8	3.5		4.8	3.2		
70	2'-ETHYLACETOPHENONE	2142645	A		2.0										5.8*		4.9*				
71	2-ETHYLHEXANOIC ACID	149575		-1.0			5.0		3.0	5.6	2.6	3.6	5.7	5.8		3.9	2.9	4.2			
72	M-TOLUIC ACID	99047					4.0		3.0	2.6	2.6		4.7	5.8			1.9	4.2	3.2		
73	P-TOLUIC ACID	99949					4.0		4.0	2.6		2.6		5.8	3.8			4.2	3.2		
74	CLOFIBRIC ACID	882097					5.0		5.0	4.6		5.6	4.7	5.8		4.9					
75	+ISOPHORONE	78591						3.0	1.0	2.6	2.7			5.8	3.8	1.9	3.9	1.2	2.2		
76	BN-BUTYL-ISOBUTYLPHTHALATE	17851535										5.6	3.7	5.0			2.9				
77	2,6-DIMETHYLBENZOIC ACID	632462											1.7	5.8		2.9		4.2	2.2		
78	1,5-HEPTADIENE-3,4-DIOL	51945983											4.7	5.8				5.2			
79	2-(2-BUTOXYETHOXY)ETHANOL (A DIETHYLE	112345					3.0	4.3		3.6	2.7	5.6	5.8		4.8	4.9	1.9	3.2	4.2		
80	3-METHYL-2-BUTEN-1-OL	556821										5.7				3.9		4.2		1.0	
81	BENZORESORCINOL	131566											5.7					1.2			
82	XCAPRIC ACID	334485		0.0			4.0			3.6		4.6	5.7	4.8		3.9		4.2			
83	XTRIBUTYL PHOSPHATE	126738		1.0		1.0	3.0		5.0	3.6*		4.6*	5.7	4.8				3.2*		2.0	-0.0
84	XAZELAIC ACID	123999			2.0	1.0	5.0	4.0		3.6	4.6*	3.6	5.7	4.8	3.8*	3.9	4.9*		2.2*	2.0	
85	XPHTHALIC ACID	88993			0.0			3.8			2.6*	5.6	5.7	4.8	3.8	2.9*			2.2		
86	XLAURIC ACID	143077				4.0		4.0*		3.6*			5.7	2.8*	3.1*	3.9*	3.9*	5.2	4.2	3.0	
87	SUBERIC ACID	505486						3.8*			3.6		5.7		2.8	2.9	2.9				1.2
88	XOLEIC ACID	112801								3.6			5.7					3.2			
89	2-CYCLOPETEN-1-ONE	930303											5.7								
90	DICYANOHEXANE	111693											5.7								

* SEE LAST PAGE OF TABLE

(Continued)

TABLE 9. (Continued)

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COMBINED CONCENTRATE REPORT(PART I.4)

	COMMON NAME	CAS NO.	RELATIVE SIZE																	
			*V1C	V1X	T28	T1C	T1X	T1Y	T4C	T4X	M2C	N2C	P2C	P2K	O2C	O2K	S2C	S2K	X1C	X1X
91	XATRAZINE	1912249										5.7			2.9					
92	1H-IMIDAZOLE-2-CARBOXALDEHYDE	10111087	-1.0								5.6		3.0			1.9				
93	XN-OCTANOL	111875		3.0							5.6		4.0			0.9*				
94	CIS-2-METHYLCYCLOPENTANOL	25144052			4.0		5.0				5.6						0.2			
95	XVALERIC ACID	109524				4.0	1.0		2.6	4.6	5.6	4.7	2.0	2.0	3.9	3.9	3.2	2.2		
96	XDICHLORACETIC ACID	79436				5.0	3.0	4.0		3.6	5.6		2.0	2.0		1.9	3.2	4.2		
97	XTRIETHYL PHOSPHATE	78400				3.0		4.0	3.6		5.6		3.0		1.9					
98	5,6,7,7A-TETRAHYDRO-4,4,7A-TRIMETHYL-2(4	15356748				4.0	3.0			2.6	5.6	2.7	4.0		4.9	3.9				
99	3-METHYL-2-BUTENOIC ACID	541479						2.0		2.6	5.6			0.3		2.9	3.2			
100	3-METHOXYPENTANE	36839675						3.0			5.6									
101	TRIPROPYLENE GLYCOL, METHYL ETHER	400							2.0	3.6	5.6			3.0						
102	TRIPROPYLENE GLYCOL, METHYL ETHER	403							2.6		5.6		4.0	3.9						
103	6-METHYL-2-HEPTANONE	928687							0.6		5.6		4.0		3.0		2.2			
104	XPROPYL ALCOHOL	71238									5.6									
105	2,2-DIETHYLPROPYLENE GLYCOL	115764									5.6									
106	AMYL CHLORIDE	543599									5.6		4.0							
107	3,5-DIMETHYLCYCLOHEXANOL	5441521									5.6	1.7			2.9		2.2			
108	1-METHYL-3-CYCLOHEXEN-1-OL	33061164									5.6									
109	CYCLOHEXYL FORMATE	4351546									5.6		1.0				2.2			
110	1,1,1-TRICHLORO-2-PROPANONE	918003									5.6									
111	X2-CHLORO-1,1-DIETHOXYETHANE	621625						5.6												
112	XDICAMBA	1918009		0.0		4.0			2.6	5.6		4.7		1.1			2.2	3.2		
113	XISOBUTYRIC ACID	79312								5.6				3.3						
114	2-METHYL-3-BUTEN-2-OL	115184							2.6		4.6	9.3	4.0		3.9					
115	XBENZALDEHYDE	100527		2.2	1.0	3.0	4.0	5.3	2.0	2.0*	4.6	4.7	3.0	3.0*	4.9	1.9*	2.2	1.2*		
116	DIETHYLENE GLYCOL, BUTYL ETHER	431						1.0				1.7			3.3		5.2			
117	3,3,3-TRICHLOROPROPENE	2233003							-0.4						3.9			5.2		
118	2-ETHYL-3-METHYLFUMARIC ACID	28098608												3.0			9.2	4.2		
119	ETHYL LACTATE	97643															5.2			
120	DIACETYLBENEZENE	1009616															5.2			
121	ALDOL	107891															5.2			
122	X1-(ETHENYLOXY)BUTANE	111342															5.2			
123	6-PROPYL-BETA-RESORCYLIC ACID	4707500																5.2		
124	4-ISOPROPYL-O-PYROCATECHUIC ACID	19420612																5.2		
125	N-TRIETHYLENE GLYCOL, MONOETHYL ETHER	112505				1.0				0.6			1.0	9.1		3.9				
126	DIPROPYLENE GLYCOL, METHYL ETHER	425							2.7	3.0	1.6	4.7	2.0	9.1						
127	METHYL MYRISTATE	124107	1.0		1.0			5.0							2.9*					
128	METHYL STEARATE	112618	1.3		2.0		2.0*	5.0												
129	DIOCTYL ADIPATE	123795	0.0	0.0			2.0*	5.0*	0.4*	2.6*	3.6*		3.0*		1.9*	0.9*			3.6	
130	X*%STYRENE	100425		0.0	1.0			5.0	-1.4*				-0.2*	0.1*	3.9		0.2*			
131	1,3-DIETHYL BENZENE	141935 A		3.0	3.0			5.0*		2.6*				1.0*	4.9	-0.1				
132	1,4-DIETHYL BENZENE	105055 A		4.0	3.0			5.0*		2.6*				1.0*	4.9	0.9				
133	1,2-DIETHYL BENZENE	135013 A		3.3	2.0			5.0*		1.6*				1.0*	4.9	0.9				
134	X*%DIOCTYLPHTHALATE	117840		3.0	2.0			5.0*				1.7*		2.0*						
135	ETHYL PALMITATE	628977 A		3.0	1.0			5.0*	1.4	2.6*.				4.0*		4.9		1.2		0.2

* SEE LAST PAGE OF TABLE

(Continued)

TABLE 9. (Continued)

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COMBINED CONCENTRATE REPORT(PART I.A)

	COMMON NAME	CAS NO.	*	RELATIVE SIZE																	
				V1C	V1X	T2B	T1C	T1X	TLY	T4C	T4X	N2C	N2C	P2G	PEX	O2G	OEX	S2G	S2X	K1C	X1X
136	METHYL-3,5-DIMETHYL BENZOATE	25081394				3.0			5.0												
137	2-METHOXY-3-METHYLCROTONIC ACID	98973185					1.0	3.0	5.0		3.6	2.6			1.0		2.9		4.2		
138	XDIBROMOCHLOROMETHANE	124481					3.1		5.0	-0.4		4.6	4.7	2.0				1.2			
139	2-CYCLOHEXENONE	930687					4.1		5.0			4.6	4.7	4.0							1.2
140	2,3,5,6-TETRACHLOROTEREPHTHALIC ACID	2136790						5.0	5.0		3.6										
141	XBM-XYLENE	108383							5.0	0.6						1.9		2.2			
142	X3-CHLORO-2-METHYL PROPENE	563473							5.0												
143	X*8O-DICHLORO BENZENE	95501							5.0			2.6		0.0		0.9		2.2			
144	X**$HEXACHLORO-1,3-BUTADIENE	87683							5.0				0.7								
145	P-METHYLSULFONYL TOLUENE	3185997							5.0												
146	1,1,3,3-TETRAMETHYL-2-INDANONE	5689123							5.0												
147	2,3-DIMETHYL-2-BUTANOL	594605							5.0				3.7					2.2			
148	METHYL HEPTANOATE	106730							5.0												
149	PHENYL ACETIC ACID, METHYL ESTER	101417							5.0												
150	DI-(2-BROMOETHYL)ETHER	5414197							5.0												
151	1-ISOCYANO-4-METHYLBENZENE	7175475							5.0												
152	SULFONYLBIS(4-CHLOROBENZENE)	80079							5.0												
153	2-ETHYL-4-METHYL-1-PENTANOL	106672					3.0	5.0													
154	3-METHYLCYCLOPENTANONE	1757422					4.0	5.0							1.5		1.9		2.2	8.0	
155	XCAPROIC ACID	142621		-1.0		1.0	5.0	4.0	2.0	-4.6	4.6	3.6	4.7	4.0	3.0	4.9	3.9	3.2			1.2
156	X**PHENOL	108952			2.0		5.0	4.0	3.0	3.6	3.6	2.6	3.7			0.9	3.0				
157	X$1,1,2,2-TETRACHLOROETHANE	79345				5.0	5.0*	4.0*		0.0*		1.0*						0.2*	1.2*	5.0	
158	XN-HEPTANOIC ACID	111148					5.0	4.0	1.0	4.6	3.6	3.6	3.7	2.0	1.5	3.9		2.2	2.2		0.2
159	2,3,3-TRICHLORO-2-PROPENOIC ACID	2257354					5.0	4.0	3.0		3.5			4.0	3.1				4.2		
160	N-HYDROXYPHTHALAMIDE	524389					5.0	4.0			3.6										
161	1-ETHOXY-1-METHOXYETHANE	10471144					5.0														
162	1-1-DIMETHOXYPROPANE	4744109					5.0														
163	~~2,3-DIMETHYLMALEIC ACID~~ SEE NO. 14	~~25713375~~					~~5.0~~	~~4.0~~													
164	ISOPROPYL BENZOATE	939480					5.0														
165	1,1-BIS(4-ETHYLPHENYL)ETHANE	10224916	A		5.0						2.6*				3.1*		2.9*				2.2
166	4-ETHYLSTYRENE	3454077	A		5.0	1.0			3.0*		3.6*				4.9*	4.0	4.1				0.2
167	XSTILBENE (CIS OR TRANS, SEE NO. 411)	588590	A		5.0										1.8*						
168	2-HEPTENYLBENZENE	26447632	A		5.0										2.0*		0.9				
169	X2-METHYLNAPHTHALENE	91576	A		5.0			2.0		-1.4	1.6	0.6	1.7	0.0	4.0*	0.9	2.9	0.2			-0.0
170	XBIPHENYL	92524	A		5.0	1.0			3.0	0.6	2.6		2.7	-0.2	4.3*	2.9	4.0	0.2	-0.0		
171	2-METHYL BIPHENYL	643583	A		5.0						3.6*		1.7		4.3*						0.2
172	3,4'-DIMETHYL-1,1'-BIPHENYL	7383906	A		5.0																
173	XSTILBENE OXIDE	17619975	A		5.0						1.6*				4.0*		2.9*				1.2
174	1,1-BIS(M-ETHYLPHENYL)ETHANE	1027	A		5.0																
175	XCYCLOPROPYL METHYL KETONE	765435				5.0							3.7			1.9					
176	2-METHYLCYCLOPENTANOL (GEOMETRY UNKNOWN)	24070777				5.0						4.6		3.0			1.1				2.2
177	XMETHYL BUTYLKETONE	591786				5.0						4.6*		2.8*				2.2*		4.0	
~~178~~	~~CARBONIC ACID~~	~~455~~																		~~5.0~~	
179	2-HEXANEAMINE	5329793																		5.0	
180	2,4-HEXADIEN-1-OL	111284																		5.0	

* SEE LAST PAGE OF TABLE

(Continued)

TABLE 9. (Continued)

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COMBINED CONCENTRATE REPORT(PART I.A)

	COMMON NAME	CAS NO.	*	V1C	V1X	T2B	T1C	T1K	T1Y	T4C†	T4K†	N2G	N2C	P2C	P2X	O2C	O2X	S2C	S2X	X1C	X1X
				RELATIVE SIZE																	
181	DIETHYL CARBINOL	584021								1.8*		2.6*	5.0	3.9		3.1		4.3		2.0	
182	XBENZYL ALCOHOL	100516								2.6	3.6	4.6	5.0						1.2		
183	2,3-DIHYDRO-4-METHYLFURAN	34314835								2.6		1.6				4.9		2.5			
184	ETHYLBENZALDEHYDE	53951501	A		4.0	2.2			4.0*		3.6*				4.9*	0.9	3.9*		0.0*		0.0
185	2*,3*-DIMETHYLACETOPHENONE	2142714	A												3.8*		4.9*		1.2*		
186	3-ETHYLSTYRENE	7525624	A		4.0	2.0					3.7*			0.0	3.9*	4.9	4.0*				0.2
187	ETHYL MYRISTATE	124061	A		4.0				4.0*		1.6*				3.0*	4.9	2.9*		1.2*		-0.0
188	DECAHYDRO-2,3-DIMETHYLNAPHTHALENE	1008806				2.0			3.0							4.9					
189	2,3-DIMETHYLBENZOIC ACID	603792					4.0						3.7	4.0	1.0	4.9		3.2			
190	X*(2,4,5-TRICHLOROPHENOXY)ACETIC ACID	93765					1.0		3.0	-0.4			3.7			4.9					
191	3,4-DIMETHYL-2,5-FURANDIONE	766392									2.6		3.7			4.9					
192	1,2,3-TRIMETHYL-4-PROPENYLNAPHTHALENE (T	26137531	a								3.6*	0.6	1.7				4.9*		3.2*		3.2
193	2-HEXANOL	626937												2.0	2.0	4.9				1.0	
194	DIETHYLENE GLYCOL, MONOMETHYL ETHER (C	111900													2.0	4.9	3.9	4.2	0.2		
195	3-ETHYL-4-METHYL-1H-PYRROLE-2,5-DIONE	20189428														4.9					
196	2,3-dimethylmaleimide	17825864														4.9					
197	5,6-DIMETHYL-1-INDANONE	16440974														4.9					
198	4A,5,6,7,8,8A-HEXAHYDRO-4A,8A-DIMETHYL-2	13485660														4.9	4.9				
199	XO-CRESOL	95487															4.9				
200	4,4-DIMETHYLDIHYDROFURANONE	13861977										4.9									
201	3-METHYLPENTAN-3-OL	77747		0.0				4.0	3.0				2.7*	4.9				2.2*	2.2		
202	2,5-HEXANEDIONE	110134					3.0	3.0		0.6		2.9		4.9	1.0	3.9		4.2	3.2		
203	TRIPROPYLENE GLYCOL, METHYL ETHER	401								2.6	3.6	4.6		4.9	4.0						
204	TRIPROPYLENE GLYCOL, METHYL ETHER	402								2.6	3.6	4.6		4.9	3.0						
205	VERATRIC ACID	93072			1.0					1.6					4.0			2.2	3.2		
206	X1-METHYLNAPHTHALENE	90120	A		4.0				1.0*		0.6*		1.7	0.0	4.0*	0.1	2.9*	0.0			
207	(1-NITROPROPYL)BENZENE	5279141			4.0										4.0*						
208	2,5-DIMETHYLBENZALDEHYDE	5779942	A		4.0	1.0			3.0*						4.0*	2.9	3.9*		0.2		1.2
209	3-METHYLBIPHENYL	643936	A		1.0										4.0*						
210	2-BUTOXYETHANOL	111762					3.0	3.0		0.6	0.6				4.0		2.1		2.2		
211	ETHYL LAURATE	106332	A						4.0*		1.6*				4.0*	1.9	3.9*		1.2*		
212	2-ETHYL INDAN	56147630	A												4.0*						
213	2,2,5,7-TETRAMETHYL TETRALIN	23342258	A												4.0*						
214	BENZYL METHYL KETONE	103797													4.0		3.9	1.2			
215	PALMITOLEIC ACID	2091294		1.0						2.6*			4.7	4.0			1.9	4.2	2.2		
216	3,5-DIMETHYLBENZOIC ACID	499069			1.0	1.0				2.6		2.6		4.0	2.0*		3.9*	3.2	2.2*		
217	DIISOBUTYL KETONE	108838			2.0									4.0							
218	2,2,6-TRIMETHYL-1,4-CYCLOHEXANEDIONE	20547993						3.0		2.6	2.7	4.6		4.0	3.0	3.9	3.9	4.2	2.2		
219	2,4,6-TRIMETHYLBENZOIC ACID	480637							2.0	2.6		1.6		4.0		2.9		2.2			
220	5-METHYL-2-HEPTANOL	54630501							4.0					4.0							
221	ORTHO-TOLUIC ACID	118901								2.6		3.6	3.7	4.0		2.9		4.2	3.2		
222	XHYDROCINNAMIC ACID	501520								3.6	2.6		3.7	4.0							
223	3,4-DIMETHYLBENZOIC ACID	619045								3.6				4.0		3.9		3.2			
224	ISO-HEXANOIC ACID	646071										2.6	2.7	4.0	2.0	1.9	1.9				
225	HEXAHYDROBENZOIC ACID	98895										3.6		4.0	2.0				1.2		

* SEE LAST PAGE OF TABLE

(Continued)

TABLE 9. (Continued)

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COMBINED CONCENTRATE REPORT(PART I.A)

	COMMON NAME	CAS NO.	RELATIVE SIZE																	
			V1C	W1X	T2B	T1C	T1X	T1Y	T4C†	T4X†	M2C	N2C	P2C	P2K	O2C	O2X	S2C	S2X	X1C	X1X
226	%2-PHENYLISOPROPANOL	617947									3.6	4.7	4.8	3.8						
227	1-(2-METHOXY-1-METHYLETHOXY)-2-PROPANOL	20324327										2.7	4.8							
228	4-METHYLHEXANOIC ACID	1561111											4.8		0.9		2.2			
229	3-METHYLPENTANAL	15877573											4.8							
230	~~ISOBUTYLCYCLOHEXANE~~	~~1670984~~											~~4.8~~							
231	2,2-DIMETHYL-1-PENTANOL	2370129											4.8				-0.8			
232	2-(2-METHOXY-1-METHYLETHOXY)-2-PROPANOL	55956224											4.8							
233	1-(ETHENYLOXY)HEXANE	5363644											4.8		2.9		4.2			
234	FENCHYL ALCOHOL	1632731											4.8							
235	%MENTHOL	89781											4.8							
236	1-(TRIMETHYLOXIRANYL)ETHANONE	15120997											4.8							
237	%ENDO-BORNEOL	507700											4.8							
238	1,2 3,5-BIS-O-(1-METHYLETHYLIDENE)-ALPHA	20881043											4.8							
239	4-NONANOL	5932796											4.8							
240	OCTAHYDRO-4A,5-DIMETHYL-3-(1-METHYLETHYL	55332020											4.8							
241	PHTHALIDE	87412											4.8				2.8			
242	NONADECANOL	52783434											4.8							
243	TRIPROPYLENE GLYCOL, METHYL ETHER	404											4.8							
244	5,5-DIMETHYLDIHYDROFURANONE	3123975							2.6				2.8		2.9		4.8	3.2		
245	%+$BIS(2-ETHYLHEXYL) PHTHALATE	117817	2.6			3.0			4.6*		4.6*	4.7*	4.1*	2.8*	3.9*	4.8*				3.2
246	ANISIC ACID	100094		0.0				4.0	3.6	3.6		4.7	3.8	2.8*		2.9*	2.2			
247	N-BUTYLBENZENESULFONAMIDE	3622842		-1.0		2.0						4.7	3.8							
248	5,6,7,7A-TETRAHYDRO-4,4,7A-TRIMETHYL-2(4	17092921				3.0			3.6			4.7	3.8	3.8			3.2			
249	1,3-DICHLORO-2-METHYLBUTANE (A DICHLO	23010073							1.6		4.6	4.7	3.8				0.2	2.2		
250	DIPROPYLENE GLYCOL, METHYL ETHER	426							1.7	3.8	3.7	4.7	2.8	3.8						
251	5,5-DIMETHYL-2-FURANONE	20019641							2.6		4.6	4.7					3.2			
252	%TCA (TRICHLOROACETIC ACID)	76039										4.7					4.2			
253	DICHLOROPHENOXYACETIC ACID (ISOMER UNKNO	711										4.7								
254	PIVALIC ACID	75989										4.7	2.8				4.2			
255	3-CHLOROCYCLOPENTENE	96402										4.7								
256	6-(ACETYLOXY)-2-HEXANONE	4305264										4.7						-0.8		
257	6,7-DODECANEDIONE	13757909										4.7					4.2			
258	DIETHYL PENTYL PHOSPHATE	28195088										4.7								
259	7-TRIDECANONE	462180										4.7								
260	%LAURYL ALCOHOL	112538										4.7	2.8				3.2	2.5		2.2
261	N,N,4-TRIMETHYLBENZENESULFONAMIDE	599699										4.7								
262	ISOPROPYL HYDROPEROXIDE	3031752										4.7								
263	DIISOOCTYLPHTHALATE	27554263								4.7										
264	3,4-EPOXY-2-HEXANONE	17257817	2.0								4.6*						2.2*	2.2*		
265	%+$DIHEXYL PHTHALATE	84753	0.0								4.6									
266	%1,4-DIOXANE	123911				3.0*					4.6*	3.7*			1.9*	1.9*			4.0	
267	LEVULINIC ACID	123762				2.0	4.0	3.0	3.6		4.6	2.7	2.8	2.8	2.9	2.9	3.2	4.2		
268	1-HEPTEN-4-OL	3521913					3.0				4.6						3.2			
269	2-METHYL-1-PENTEN-3-OL	2080075					4.0				4.6						4.2			
270	N,N-DIETHYL FORMAMIDE	617845							2.6	2.6	4.6				0.9		3.2	1.2		

(Continued)

TABLE 9. (Continued)

COMBINED CONCENTRATE REPORT(PART I.A)

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	COMMON NAME	CAS NO.		RELATIVE SIZE																	
			*	VIC	VIX	T20	T1C	T1X	T1V	T4C	T4X	M2C	NEC	P2C	P2X	O2C	O2X	S2C	S2X	X1C	X1X
271	2-METHYL-2-HEPTANOL	625252									0.6	4.6						1.2			
272	3,5-DIMETHOXYPHENOL	508992										4.6									
273	%AMOBARBITAL	57432										4.6									
274	%PENTABARBITAL	76744										4.6									
275	TRANS-9-HEXADECENOIC ACID	373499										4.6						3.2			
276	PETROSELINIC ACID	593395										4.6									
277	%CYCLOHEXYL BROMIDE	108858										4.6		1.0				0.2	2.2		
278	5-METHYL-3-HEXANOL	623552										4.6							1.2		
279	2-METHYL-2-BUTEN-1-OL	4675870										4.6		3.0				2.2			
280	5-ETHYL-2-HEPTANOL	19780406										4.6									
281	3-METHOXY-1,3,4-HEXATRIENE	53783883										4.6									
282	2-METHYL-2-ISOBUTYLOXIRANE	53897317										4.6									
283	1-METHYLHEXYLHYDROPEROXIDE	762469										4.6									
284	2-BUTYL-3-METHYLOXIRANE	14925963										4.6									
285	2-METHOXY-4-METHYL-2-PENTENOIC ACID, MET	56009360										4.6	3.7								
286	2,3,4-TRIMETHYL-3-PENTANOL	3054928										4.6									
287	1-ISOCYANONAPHTHALENE	1984049										4.6									
288	N-TERT-BUTYL-3-METHYLBENZAMIDE	42498339										4.6									
289	4,5-DIETHYL-2,3-DIHYDRO-2,3-DIMETHYLFURA	54244892										4.6									
290	4,7-DIMETHYL-1,3-ISOBENZOFURANDIONE	5463503										4.6									
291	2,5-DIMETHYL-2-HEXANOL	3730607										4.6									
292	%+BUTYL BENZYL PHTHALATE	85687										4.6	3.7								
293	PROPYLOXIRANE	1083141										4.6									
294	%CYCLOHEXYL ACETATE	622457										4.6	9.7	8.8				1.2			
295	%(ETHOXYMETHYL)OXIRANE	4016119										4.6									
296	4-HEPTANONE	123193						4.6*								2.9*	0.0*	1.2*		4.0*	
297	PHENOXY ACETIC ACID	122598					4.0				4.6										
298	%ETHOSUXIMIDE	77678						3.0		2.6	4.6						3.9		3.2		
299	2-METHOXY-4-METHYL-2-PENTENOIC ACID	1009						4.0	4.0		4.6	2.6			1.0	2.9	3.9		4.2		
300	4,6-DIMETHYL OCTANOIC ACID	2553968								4.6											
301	O-CRESYL ACETATE	533186								3.6	4.6										
302	3-HYDROXYNONANOIC ACID	33796871								4.6											
303	%2,4-DIMETHOXYBENZOIC ACID	91521									4.6								2.2		
304	P-ETHYLBENZOIC ACID	619647	A								4.6*										
305	1,1-DIPHENYLETHANE	612080	A		4.2						3.7*		1.7		0.0*	0.1	-0.1*		2.2*		
306	METHYL AMYL CARBINOL	543497			1.0									3.0*				4.2*		4.0	
307	%ETHYL CARBONATE	105588							3.0					3.0				4.2			
308	5-METHYL HEXANOIC ACID	628466							2.0				2.7	3.0		2.9		4.2			
309	2-BUTYL THF	1004291								-1.4		2.6						4.2	2.2		
310	4,5-DIMETHYL-2-HEPTEN-3-OL	55956371										1.6						4.2			
311	5-METHYL-2-HEPTANONE	18217124										3.6						4.2			
312	1,3,3,7-TETRAMETHYL-2-OXOBICYCLO(2.2.1)H	15404576												3.0				4.2			
313	BUTYL ISOBUTYRATE	97870												2.0				4.2			
314	2-ETHYLCYCLOHEXANONE	4423943														3.9		4.2			
315	DIETHYLENE GLYCOL, METHYL ETHYL DIETHER	1002671																4.2			

* SEE LAST PAGE OF TABLE

(Continued)

TABLE 9. (Continued)

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COMBINED CONCENTRATE REPORT(PART I.A)

RELATIVE SIZE

	COMMON NAME	CAS NO.	*	V1C	V1X	T2B	T1C	T1X	T1Y	T4C+	T4X+	N2C	N2C	P2C	P2X	O2C	O2X	S2C	S2X	X1C	X1X
316	2-METHYLHEPTANOIC ACID	1188029																4.2			
317	1,6-HEXANEDIOL	629118																4.2			
318	2,3-DIHYDRO-4-(1-METHYLETHYL)FURAN	34314846																4.2			
319	CYCLOHEXANEHEXANOL	4354589																4.2			
320	~~2,5-DIMETHYLHEXANE~~	~~592132~~																~~4.2~~			
321	2,2,5,5-TETRAMETHYL THF	15045439																4.2			
322	%4(1H)-PYRIMIDINONE	4562270																4.2			
323	3,5-NONADIEN-7-YL-2-OL	43142434																4.2			
324	4,4,5,5-TETRAMETHYL-1,3-DIOXOLAN-2-ONE	19424294																4.2			
325	2-(1-METHYLETHYLIDENE)CYCLOHEXANONE	13747734																4.2			
326	OXACYCLOTETRADECAN-2-ONE	1725048																4.2			
327	1,1-DICHLORO-2-HEXANONE	2648591																4.2			
328	4,4-DICHLORO-3-HEXANONE	2648604																4.2			
329	DIHYDRO-5-METHYL-2(3H)-FURANONE	108292																4.2			
330	C3-DIHYDROXYBENZOIC ACID	1016																	4.2		
331	4-BUTOXYBUTYRIC ACID	55724737																	4.2		
332	%$1,2-DICHLOROETHANE	107062					3.0		2.0								4.1				
333	PENTAETHYLBENZENE	605016			4.1																
334	O-ETHYLBENZOIC ACID	28134318	A		3.0				4.0*		3.6*										1.2
335	%+$DICHLOROETHYL ETHER	111444			-1.0				4.0						0.8*		-0.1*				
336	%ETHYL BENZOATE	93890	A		4.0	1.0			4.0*						1.0*	1.9					1.2
337	ETHYL PENTADECANOATE	41114005	A		2.0				4.0*		1.6*				2.0*		1.9*				
338	ETHYL STEARATE	111615	A		2.0	1.0			4.0*		1.6*				2.0*		2.9*				
339	ANTEISOPENTADECANOIC ACID	5502943				1.0			4.0												0.2
340	%*+$P-DICHLOROBENZENE	106467				1.0	1.0		4.0	-0.4		1.6	3.7	-0.2				-0.8	2.2		
341	DIHEXYLADIPATE	110388				1.0			4.0												
342	METHYL LAURATE	111820	a			3.0			4.0*												
343	METHYL-2,4-DIMETHYL BENZOATE	23617712	a			2.0			4.0*												
344	2,3-DICHLOROANILINE	608275					3.0		4.0		1.6			1.8				1.2			
345	%$DIMETHYL PHTHALATE	131113					4.0		4.0												
346	%BENZYL CYANIDE	140294					2.0		4.0			1.6	3.7	3.8				1.2			
347	3-HEPTANOL	589822						3.0	4.0										-0.8		
348	1-CHLORO-2-METHYL-2-BUTENE	13417431							4.0												
349	NEOPENTYL CHLORIDE	753899							4.0			1.6									
350	1-BROMO-4-ETHYLBENZENE	1585075							4.0												
351	2,4,5-TRICHLOROANILINE	636306							4.0									1.2			
352	*PENTACHLOROANILINE	527208							4.0												
353	1,2,2,3-TETEACHLOROPROPANE	13116535							4.0	1.6											
354	%*+$1,2,4-TRICHLOROBENZENE	120821							4.0			1.6		-0.2				-0.8	2.2		
355	2,4-DICHLORO-1-NITROBENZENE	611063							4.0									0.2			
356	+%LINDANE (BETA ISOMER)	319857							4.0				2.7								
357	%*PENTACHLORONITROBENZENE	82688							4.0												
358	DIMETHYL AZELATE	1732101							4.0												
359	4-TERT-BUTYL-2-METHYLPHENOL	98271							4.0	-0.4							3.9	2.2			
360	4-METHYLPHENYLSULFONYL ACETIC ACID, METH	50397643							4.0												

* SEE LAST PAGE OF TABLE

(Continued)

TABLE 9. (Continued)

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COMBINED CONCENTRATE REPORT(PART I.A)

				RELATIVE SIZE																	
	COMMON NAME	CAS NO.	*	VLC	VLX	T28	T1C	T1K	T1Y	T4C†	T4K†	M2C	M2C	P2C	P2X	O2C	O2X	S2C	S2X	X1C	X1X
361	4-METHYL-1-PHTHALAZINONE	5004488							4.0												
362	2-METHYL-2-PENTANOL	590363							4.0			3.6	3.7			0.9		2.2			
363	%CAMPHOR	76222							4.0									2.2			
364	2-KETOISOCAPROIC ACID	816660							4.0		2.6				0.8						
365	PENTYLENETETRAZOLE	54955							4.0							2.9					
366	SUCCINIC ACID, DIMETHYL ESTER	106650							4.0												
367	%DIETHYL SUCCINATE	123251							4.0												
368	2,2-DIMETHYLGLUTARIC ACID	681572							4.0												
369	1-(METHYLPHENYL)ETHANONE	26444199	A						4.0*		1.6*						1.9*				
370	METHYLSULFONYL BENZENE	3112854							4.0												
371	ALLYL-1,3-DIOXANE	4528261							4.0												
372	METHYL CAPROATE	106707							4.0												
373	METHYLCAPRYLATE	111115							4.0												
374	METHYL PELARGONATE	1731846							4.0												
375	ETHYLNONENOATE	35194399							4.0												
376	METHYL CAPRATE	110429							4.0												
377	BENZONITRILE	100470							4.0					1.8							
378	PHENYLPROPIONIC ACID,METHYL ESTER	103253							4.0												
379	2,4,5-TRICHLOROPHENOXY ACETIC ACID, METH	35389440							4.0												
380	2,2-DIMETHYL-3-PENTANOL	3970625							4.0												
381	(1-ETHOXYETHYL)BENZENE	3299056	a						4.0*								3.9*		-0.8		
382	1,2-DIMETHYL-4-NITROBENZENE	99514							4.0												
383	METHYL HEPTADECANOATE (METHYL MARGARAT	1731926							4.0												
384	1-(2-BUTOXYETHOXY) ETHANOL	54446785			2.0			4.0		-0.4				1.8		3.9		2.2	1.2*		
385	2-HEXENOIC ACID	1191044					4.0	4.0	3.0						1.8						
386	METHYL N-AMYL KETONE	110430						4.0		-1.4		3.6	3.7						1.2		
387	%DALAPON	75990						4.0	3.0		2.6							3.2	3.2		
388	HENEICOSANIC ACID	2363715						4.0													
389	HEPTYL ALCOHOL	111706						4.0		1.6											
390	%BIS(2-ETHYLHEXYL) ADIPATE	103231				3.1	4.0*					3.6*	2.7*			3.9*	3.9*				
391	ADIPIC ACID, DIHEXYL ESTER	110338				3.0	4.0*	2.0*									2.9*				
392	6-UNDECANOL	23708567					4.0	3.8							2.8			-0.8			
393	P-ISOPROPYL BENZOIC ACID	536663					4.0			2.6				1.8				3.2			
394	4,4-DICHLOROBUTENOIC ACID	16502088					4.0				2.6			3.8	1.8				3.2		
395	%ANTHRANILIC ACID	118923					4.0														
396	2-METHYL-4-(2,5-XYLYL)BUTANOIC ACID	30316144					4.0														
397	2-(2-HYDROXYPROPOXY)-1-PROPANOL (A DIPRO	106627					4.0				0.6	3.6									
398	2-PHENOXYETHANOL	122996					4.0														
399	CYCLIC TETRAMETHYLENE ADIPATE	777957					4.0			3.6											
400	1-CYCLOPENTYLETHANONE	6004600					4.0									1.9		3.5			
401	(2-ETHOXY-1-METHOXYETHOXY)-ETHENE	54063182					4.0														
402	N,N*-DIMETHYLUREA	96311					4.0														
403	DIPHENYLMETHANE	101815	A		4.0						2.6*				2.3*		2.9*				
404	1,2-DIHYDRONAPHTHALENE	447530	A		4.0										2.8*		0.9*				
405	TETRAETHYLBENZENE	33637206	A		4.0						2.6*				3.8*		2.9*				1.2

* SEE LAST PAGE OF TABLE

(Continued)

TABLE 9. (Continued)

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COMBINED CONCENTRATE REPORT(PART I.A)

	COMMON NAME	CAS NO.	*	RELATIVE SIZE																	
				V1C	V1K	T2D	T1C	T1K	T1Y	T4C†	T4K†	N2C	M2C	P2C	P2X	O2C	D2X	S2C	S2K	X1C	K1X
406	1-ETHYLNAPHTHALENE	1127760	A		4.0										3.0*		1.9*				
407	1-METHYL-7-ISOPROPYL NAPHTHALENE	490653	A		4.0																
408	X3-METHYLPHENANTHRENE	832713	a		4.0										1.8*						
409	1-PHENYL TETRALIN	3018200	A		4.0						0.6*				2.0*		1.9*				0.2
410	1,1-BIS(O-ETHYLPHENYL)ETHANE	1023	A		4.0																
411	XSTILBENE (TRANS OR CIS, SEE NO. 167)	103300			4.0										3.0*		1.9*				-0.0
412	2-PHENYL TETRALIN	29422137	A		4.0						0.6*				2.5*		1.9*				1.2
413	3-ETHYLACETOPHENONE	22699703	A		4.0						2.6*						3.9*				
414	2-(ETHYLPHENYL)PROPYL METHYL ETHER	667			4.0																
415	XETHYLENE TETRACHLORIDE	127184				4.0				2.6											2.2
416	$ETHYLBENZENE	100414				2.0				1.6*						1.9*		2.5*	2.2*	4.0	
417	X$P-XYLENE	106423				3.0			3.3*							1.9		1.2	2.2	4.0	
418	(1,4-CYCLOHEXADIEN-1-YL)BENZENE	13703521																		4.0	
419	DIACETONE ALCOHOL	123422											4.0	3.0				2.5		3.0	
420	2,6,6-TRIMETHYL-1-CYCLOHEXENE-1-CARBOXAL	432257														3.0					
421	TRIETHYLENE GLYCOL METHYL ETHER	112356													3.9						
422	9-KETOCAPRIC ACID	1422260		-1.3											1.0*	3.9					
423	X*+$PENTACHLOROPHENOL	87865		0.0			1.0		2.0	1.6*			3.7		-0.2	3.9		1.2*			
424	1,3,5-TRIETHYLBENZENE	102250			3.0						2.6*				3.0*	2.9	3.9*				-0.0
425	2,6-DIMETHYL DECALIN	1618220				1.0										3.9					
426	XBUTROLACTONE	96480				3.0										3.9					
427	X*2,4-DICHLOROPHENOXYACETIC ACID, (2,4-D)	94757					1.0		3.0	2.6			3.7			3.9	2.9				
428	1,1,3-TRICHLORO-1-PROPENE	2567148					2.0			0.6		3.6	3.7	3.0		3.9		1.2	2.2		
429	SEBACIC ACID	111206									2.6				2.0		3.9				
430	2,6-DIMETHYL ACETOPHENONE	2142769	a								1.6*						3.9*				
431	2,4,5-TRIMETHYLBENZOIC ACID	528905										2.6		3.0		3.9		3.2			
432	3-HYDROXYTETRADECANOIC ACID	1961724											3.7			3.9					
433	O-ANISIC ACID	579759												3.0	1.6	3.9	2.9				
434	3-OCTEN-2-ONE	1669449												2.0		3.9					
435	DIOCTYL SEBACATE	122623												2.0		3.9					
436	2-METHOXY-3,5,5-TRIMETHYL-2-CYCLOHEXENE-	41654277														3.9	0.9		2.2		
437	PIPERIDINONE	27154434														3.9					
438	TETRAHYDRO-2-METHYL-2-FURANOL	7326467														3.9					
439	XSUCCINIC ACID	110156															3.9				
440	2-ETHOXYNAPHTHALENE	93185															3.9				
441	XN-DECYL ALCOHOL	112301												3.0			1.9	2.2			
442	1,2,4-TRIETHYLBENZENE	877441	a		3.0						2.6*				3.0*	1.9	2.9*				-0.0
443	TETRALIN	119642	A		3.0	1.0			2.0*		1.6*		1.7	-0.2	3.0*	1.9	2.9*	0.0			
444	DIVINYLBENZENE	1321740	A		2.0						1.6*				3.0*	1.9					
445	P-ETHYLBENZALDEHYDE	4748781	A		2.0						3.6*				3.0*	2.9			-0.0*		
446	2*-METHYLACETOPHENONE	577162	A		1.0								2.7		3.0*		1.9				
447	1-METHYL TETRALIN	1559815	A		2.0						1.6*			-0.2	3.0*			-0.0			
448	1,1-DIMETHYL INDAN-4-CARBOXYLIC ACID, ET	55591123	A		1.0										3.0*		2.9*				3.2
449	2-ACETYLOXYACETOPHENONE	2243358	a			2.0									3.0*						
450	3-METHYL-2-CYCLOHEXEN-1-ONE	1193186					2.3			2.6				0.0	3.0		1.9	2.2	2.2		

* SEE LAST PAGE OF TABLE

(Continued)

TABLE 9. (Continued)

COMBINED CONCENTRATE REPORT(PART I.A)

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	COMMON NAME	CAS NO.	*	RELATIVE SIZE																	
				V1C	V1X	T2B	T1C	T1X	T1Y	T4C†	T4X†	M2C	N2C	P2C	P2X	O2C	O2X	S2C	S2X	X1C	X1X
451	2',4'-DIMETHYLACETOPHENONE	89747	A						3.0*			3.6			3.0*		2.5*		0.5*		
452	%2-ETHYL NAPHTHALENE	939275	A								1.6*				3.0*		2.9*				0.2
453	3-METHYL VALERIC ACID	105431										3.6		2.8	3.0	0.9	2.9				
454	2-METHYL INDAN	824635	A										1.7		3.0*	1.9					
455	2,2-DIMETHYL-3,5-DECADIYNE	95682730													3.0						
456	5-METHYL INDAN	874351	A												3.0*			-0.8			
457	2,5-CYCLOHEXADIENYLBENZENE	4794852													3.0						
458	ALPHA-METHYLSTILBENE	833818	A												3.0*						
459	2,3,4,5,6-PENTAFLUORO-N-(2-PHENYLETHYL)B	38842147													3.0						
460	4,4'-DIETHYLBIBENZYL	57364791	A												3.0*						
461	DIPROPYLENE GLYCOL METHYL ETHER (1-(2-	13429077													3.8						
462	3-PROPYLCYCLOPENTENE	34067759													3.8						
463	2-HENDECANOL	1653301													3.8		1.9				
464	1-UNDECANOL	112425													3.8			2.2			
465	HEXYL BENZOATE	6789884													3.8						
466	PENTYL BENZOATE	2049969													3.8						
467	BENZOTHIAZOLE	95169		1.8			3.0*		3.0	2.6*				3.8*				3.2*			
468	%*$P-CHLOROPHENOL	106489					2.8		3.8	2.6				3.8		1.9					
469	4-METHYLPHTHALIC ACID	4316238						2.8					3.7	3.8					1.2		
470	%2-NAPHTHOIC ACID	93094								1.6			2.7	3.8				2.2			
471	%*+$2,4-DICHLOROPHENOL	120832								-0.4			2.7	3.8							
472	1,2,3,3-TETRACHLORO-1-PROPENE	28589859								-1.4		3.6		3.8				2.2			
473	1-METHYL-4-(1-METHYLETHYL)-7-OXABICYCLO(	470677								1.6			3.7	3.8							
474	%CAFFEINE	58082								3.7	2.8		3.7	3.8							
475	2-METHYL VALERIC ACID	97610										1.6	1.7	3.8	1.3	0.9	0.9				
476	1-(4,5-DIETHYL-2-METHYL-1-CYCLOPENTEN-1-	62338243										3.6		3.8							
477	FENCHONE	1195795											3.7	3.8							
478	3-OCTENOIC ACID	1577191												3.8							
479	1-PHENYLBUTYRIC ACID	1821121												3.8							
480	2-HYDROXYTETRADECANOIC ACID	2507553												3.8							
481	3-METHYLPHTHALIC ACID	37102742												3.8							
482	4-METHYL-3-PENTENAL	5362505												3.8							
483	%CINEOLE	470826												3.8							
484	3-ETHOXY-3-METHYL-2-BUTANONE	36687997												3.8							
485	ISOPROPENYLBENZENE	98839												3.8							
486	6-METHOXY-2-HEXANONE	29006006												3.8							
487	2,[illegible]EPTANEDIONE	7307820												3.8							
488	2-[illegible]LOOCTYL-2-PROPANOL	16624069												3.8							
489	METHYL 2,2,3-TRIMETHYLCYCLOPENTYL KETONE	17983221												3.8							
490	THIOHEXANOIC ACID, S-BUTYL ESTER	2432793												3.8							
491	3-ETHOXY-3-METHYL-1-BUTYNE	7740694												3.8		2.9		3.2			
492	5-(PENTYLOXY)-2-PENTENE	56052858												3.8		1.9					
493	2-ETHYL-3-METHYLOXETANE	53778624												3.8							
494	2-METHYL-2-PROPYL-1,3-DIOXOLANE	4352981												3.8							
495	2-ETHYL-1,3,2-DIOXABOROLANE	10173383												3.8							

* SEE LAST PAGE OF TABLE

(Continued)

TABLE 9. (Continued)

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COMBINED CONCENTRATE REPORT(PART I.A)

	COMMON NAME	CAS NO.	RELATIVE SIZE																	
			V1C	V1K	T2B	T1C	T1K	T1Y	T4C†	T4K†	M2C	N2C	P2C	P2K	O2C	O2K	S2C	S2X	X1C	X1K
496	BORNYL 2,5-DIKETONE	4230324											3.8							
497	7,7-DIMETHYL-11-DODECEN-2-ONE	35194220											3.8							
498	METHYL 9-OXODECANOATE	2575077											3.8							
499	CYCLOOCTANEPROPANOL	16782302											3.8							
500	CYCLOHEXYL METHYL KETONE	823767											3.8			0.9				
501	P-ISOPROPYLBENZALDEHYDE; CUMINALDEHYDE	122032											3.8		2.9		0.2			
502	2,3 5,6-DI-O-ISOPROPYLIDENE-ALPHA-D-TALO	23262784											3.8							
503	1-TERT-BUTYL-4-ETHOXYBENZENE	17269942											3.8							
504	5-METHYL-1(3H)-ISOBENZOFURANONE	54120648											3.8				3.2			
505	9-OCTADECENAL	5090415											3.8							
506	4-METHYL-3-HEPTEN-2-ONE	22319251											3.8				2.2			
507	6-METHOXY-2-METHYL-3-HEXANONE	17429059											3.8							
508	2,6-DIMETHYL-3-HEPTANOL	19549736											3.8							
509	2-(2-METHOXY-1-METHYLETHOXY)-1-PROPANOL	55956213											3.8							
510	AMYL BUTYL PHTHALATE	1018											3.8							
511	2-ETHYL-2-ISOBUTYL-1,3-DIOXOLANE	935455											3.8							
512	ELAIDIC ACID	112798	2.8		1.0							3.7*					3.2*	1.2		
513	P-(1-HYDROXY-1-METHYLETHYL)ACETOPHENONE	54549723	0.0									3.7					2.2			
514	%P-CHLOROBENZOIC ACID	74113		3.8				3.0				3.7	2.8							
515	3,4-DICHLOROBENZOIC ACID	51445		0.0				3.0				3.7					2.2			
516	2,2,6-TRIMETHYLCYCLOHEXANONE	2408379				2.0		3.6		1.8	3.6	3.7	2.8	2.8	1.9	1.9	2.2	0.2		
517	2,3-DIMETHYLBUTYRIC ACID	14287617						2.8		3.6	2.6	3.7	1.8	2.8	1.9	1.9	3.2	2.2		
518	DICHLOROISOPROPYL ETHER	108601						1.0				3.7								
519	PENTACHLOROCYCLOPROPANE	6262517							1.6			3.7								
520	2,3-OCTANEDIONE	585251							2.6	2.6		3.7				1.9		-0.8		
521	~~1-ETHYL-2,3-DIMETHYLCYCLOHEXANE~~	~~7058051~~							~~0.6~~			~~3.7~~								
522	BUTYLBENZOATE	136607									2.6	3.7	0.8							
523	2-PHENYLBUTYRIC ACID	90277										3.7								
524	3-METHOXYBENZOIC ACID	586389										3.7	1.8							
525	2,6-DICHLOROBENZOIC ACID	50793										3.7								
526	UNDECANEDIOIC ACID	1852046										3.7		2.8		2.9				
527	%CHLOROBROMOMETHANE	74975										3.7								
528	TRICHLOROPHENOXYACETIC ACID (ISOMER UNKN	713										3.7								
529	3-BROMO-1,1-DICHLOROPROPANE	36668458										3.7								
530	%TERT-PENTYL ALCOHOL	75854										3.7								
531	5-METHYLHEXANOL	1868395										3.7								
532	CIS-3,4,4-TRIMETHYL-5-OXO-2-HEXENOIC ACI	14919541										3.7				2.9				
533	ETHYLENE GLYCOL, MONOMETHYL ETHER	109864										3.7								3.2
534	4-ISOPROPYLCYCLOHEXANOL	4621049										3.7								
535	4-METHYL-3-HEPTANOL	14979396										3.7								
536	SEC-BUTYLISOPROPYL ETHER	18641811										3.7								
537	%2-PROPENYL HEXANOATE	123682										3.7								
538	CYCLOPENTANONE	120923										3.7								
539	VINYL BUTYRATE	123206										3.7								
540	TETRAHYDRO-5-METHYL-2-FURANMETHANOL	54774286										3.7					2.2			

(Continued)

TABLE 9. (Continued)

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COMBINED CONCENTRATE REPORT(PART I.A)

	COMMON NAME	CAS NO.	VIC	VIX	T2B	T1C	T1X	T1Y	T4C†	T4K†	N2C	N2C	P2C	P2X	O2C	O2X	S2C	S2X	X1C	X1X
541	OCTAHYDRO-2,2,4,4,7,7-HEXAMETHYL-1H-INDE	54832836										3.7								
542	OCTYL ACRYLATE	2499594										3.7					3.2			
543	%N-METHYL-2-PYROLIDONE	872504					1.0		3.7	3.6										
544	4-KETOISOHEPTANOIC ACID	41654040		1.0		3.0	3.0		2.6	3.6*	3.6	2.7		2.0*		2.9*	2.2	3.2*		
545	3-METHYL-4-PENTEN-2-ONE	758872				3.0					3.6							2.2		
546	2-METHYL-2-PROPYLHEXANOIC ACID	31080372						2.0			3.6									
547	3,3-DIMETHYLBUTYRIC ACID	1070833								3.6	3.6	2.7	2.8	1.8			3.2			
548	CHRYSANTHEMIC ACID	10453891									3.6									
549	CIS-1,3-DICHLOROCYCLOHEXANE	24955633									3.6									
550	3,4-DIHYDRO-6-METHYL-2H-PYRAN	16015115									3.6									0.2
551	5-METHOXY-2-METHYL-2-PENTANOL	55724044									3.6		2.8							
552	2-VINYLCROTONALDEHYDE	20521420									3.6				1.9					
553	(1-METHYLBUTYL)OXIRANE	53229393									3.6								3.0	
554	2-HYDROXYCYCLOHEXANONE	533608									3.6									
555	5-METHYL-1-HEXANOL	627985									3.6									
556	2-T-BUTYL-2-METHYL-1,3-DIOXOLANE	6135542									3.6									
557	3-CHLORO-2-CYCLOPENTEN-1-ONE	53102140									3.6				1.3					
558	4,6,6-TRIMETHYLTETRAHYDRO-2-PYRANONE	20628368									3.6									
559	3,7-OCTADIEN-2-ONE	25172069									3.6									
560	2-HEPTENOL	33467764									3.6									
561	2-BUTOXYPENTANE	62238022									3.6									
562	ALPHA-ACETYLBUTYROLACTONE (GAMMA LACTONE	517237									3.6									
563	2-OCTEN-1-OL	18409171									3.6									
564	CHLOROACETONITRILE	107142									3.6									
565	%TERPIN	80535				3.6	2.8			0.6				2.8						
566	2-METHYLENEBUTYRIC ACID	3586581						1.0		3.6				1.8	1.9	2.9		2.2		
567	%ETHYLENE GLYCOL MONOETHYL ETHER) (OXITOL	110805							3.6							0.9				
568	3,6-DIMETHYLOCTANOIC ACID (AN ISODECANOI	4812297							3.6											
569	3-METHYL-4-PHENYLBUTYRIC ACID	7315686							3.6											
570	OCTAHYDRO-1,4A-DIMETHYL-1-PHENANTHRENE C	3650042							3.6											
571	1,3-DIMETHYL-2-(2-ISOPROPYLPHENYL)ETHYLC	6080							3.6											
572	%7-OXABICYCLO[4.1.0]HEPTANE	286204							3.6		2.6									
573	% PYRIDINE	110861							0.6	3.6										
574	%1,2-DIHYDRO-3,6-PYRIDAZINEDIONE	123331								3.6										
575	3-HYDROXYOCTANOIC ACID	14292274								3.6										
576	3,4-DIHYDROXYBENZALDEHYDE	8897								3.6										
577	2,3-DICHLOROACRYLIC ACID	8896								3.6										
578	5-OXO-HEXANOIC ACID	3128061								3.6						1.9				
579	2-(HYDROXYMETHYL)BENZOIC ACID	612204								3.6								0.2		
580	~~ACETIC ACID~~	~~64197~~								~~3.6~~										
581	TRIPROPYLENE GLYCOL, METHYL ETHER	20324338								3.6										
582	%*ANILINE	62533								3.6										
583	%2,2,2-TRICHLOROETHANOL	115208															3.3			
584	4-ACETYLMORPHOLINE	1696204				3.3														
585	2-METHYLPHENYLPROPANOIC ACID	22084895		-1.0													3.2			

(Continued)

TABLE 9. (Continued)

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COMBINED CONCENTRATE REPORT(PART I.A)

	COMMON NAME	CAS NO.	*	V1C	V1X	T23	T1C	T1K	T1Y	T4C†	T4K†	M2C	N2C	P2C	P2K	O2C	O2K	S2C	S2X	X1C	X1K
586	%TERT-BUTANOL	75650			2.0													3.2			
587	2-METHOXY-3-METHYL-2-PENTENOIC ACID	1000					3.0	3.0	3.0		2.6				1.1		2.9		3.2		
588	O-CHLOROBENZOIC ACID	118912							3.0						2.8			3.2	2.2		
589	2,5-DIMETHYLBENZOIC ACID	610720								2.6				1.0	0.0	2.9	2.9	3.2			
590	3-METHYL-2-CYCLOPENTEN-1-ONE	2758181								2.6	1.7		2.7				1.9	3.2			
591	2,4-DIMETHYL-4-HEPTANOL	19549770										1.6						3.2			
592	5-EPIDEOXYPODOCARPIC ACID	57345309											1.7			2.9		3.2			
593	2-METHYLCAPROIC ACID	4536236												0.0				3.2			
594	2,3,4,5,5-PENTACHLORO-2,4-PENTADIENOIC A	5659416												1.0				3.2	2.2		
595	2-METHYL-2-HEPTEN-4-ONE	22319240															0.9	3.2			
596	%2-ACETYLFURAN	1192627															0.9	3.2	1.2		
597	4-AMINO-3,5-DICHLOROBENZOIC ACID	56961252																3.2			
598	4-ETHYLHEXANOIC ACID	6299667																3.2			
599	%AMIBEN	133904																3.2			
600	VACCENIC ACID	693721																3.2			
601	ETHYL ISOBUTYL KETONE	623563																3.2			
602	%METHYLAL	109875																3.2			
603	3-METHYL-2-HEXANOL	2313657																3.2			
604	1-METHYL-4-METHYLENESUBERANE	23799259																3.2			
605	2,4-DIMETHYL-2-PENTENE	625650																3.2			
606	ACETYL ISOBUTYRYL	7493585																3.2			
607	~~DECALIN~~	~~493016~~																~~3.2~~			
608	1,2-DIMETHYLCYCLOHEXENE	1674108																3.2			
609	~~PENTYL TRIMETHYLENE~~	~~3614013~~																~~3.2~~			
610	4-METHOXY-1-BUTANOL	111320																3.2			
611	3,4-EPOXY-3-ETHYL-2-BUTANONE	17257828																3.2			
612	~~2,7-DIMETHYLOCTANE~~	~~1072168~~																~~3.2~~			
613	3,4-DIHYDRO-2,5-DIMETHYL-2H-PYRAN-2-CARB	1920214																3.2			
614	~~1,1,3-TRIMETHYLCYCLOHEXANE~~	~~3073663~~																~~3.2~~			
615	2-BUTYL-N-BUTYRATE	819976																3.2			
616	N-BENZOYLGLYCINE, METHYL ESTER	1205089																3.2			
617	CUMENE ISOPROPYL ETHER	24142776																3.2			
618	1,3-DIMETHOXY-2-PROPANOL	623698																3.2			
619	2-ISOPROPYL-1,3-DIOXOLANE	822833																3.2			
620	1-OXIRANYLETHANONE	4401110																3.2			
621	6,6-DIMETHYL-3,4-UNDECADIENE-2,10-DIONE	52588780																3.2			
622	TEREPHTHALIC ACID	100210																	3.2		
623	3-METHOXY-2-METHYL-2-PENTENOIC ACID	1014																	3.2		
624	3-METHOXY-1,2-BENZISOTHIAZOLE	40991386																	3.2		
625	~~%DIMETHYL SULFATE~~	~~77781~~																	~~3.2~~		
626	1-METHYL-4-(1-METHYL-2-BUTENYL)NAPHTHALE	38171970																	3.2		
627	CYCLOPENTYL BROMIDE	137439																	3.2		
628	2,2-DICHLORO-3-METHYLBUTANE	17773669																	3.2		
629	SYM-DIPHENYLETHANE (BIBENZYL)	103297	A		1.0												1.9*				3.2
630	3-HYDROXY-3-METHYL-2-BUTANONE	115220							3.0	0.6	1.8	2.6		0.0	3.1	2.1	0.9	2.5	0.2		

* SEE LAST PAGE OF TABLE

(Continued)

TALBE 9. (Continued)

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COMBINED CONCENTRATE REPORT(PART I.A)

	COMMON NAME	CAS NO.	RELATIVE SIZE																	
			V1C	V1X	T2B	T1C	T1X	T1Y	T4C†	T4X†	M2C	N2C	P2C	P2X	O2C	O2X	S2C	S2X	X1C	X1X
631	METHYL PENTADECANOATE	7132641	1.0		1.0			3.0*												
632	METHYL PALMITATE	112390	2.0		2.0		2.0*	3.0*		-0.4*				2.0*				0.2*		
633	METHYL ISOPALMITATE	5129602	0.0					3.0												
634	DIBENZOFURAN (DIPHENYLENE OXIDE)	132649				1.0		3.0					-0.2							
635	2,2-DICHLOROBUTYRIC ACID	13023002					2.0	3.0								0.9		2.2		
636	2-ETHYLHEPTANOIC ACID	3274291						3.0												
637	M-CHLOROBENZOIC ACID	535808						3.0	2.6											
638	4-CHLOROPHENYL ACETATE	876277						3.0			2.6									
639	2,3,4,6-TETRACHLOROPHENOL	938227						3.0												
640	XCHLOROBENZENE	108907						3.0	-0.4			0.7					-0.8			
641	1-CHLORO-2-ETHYLBENZENE	89963						3.0												
642	PERCHLOROETHANE	67721						3.0					0.8							
643	1-BROMO-2-ETHYLBENZENE	1973224						3.0												
644	CHLOROVINYLBENZENE	622253						3.0									-0.8	0.2		
645	$1,2,3-TRICHLOROBENZENE	87616						3.0												
646	3,5-DIBROMOTOLUENE	1611923						3.0												
647	(1,2-DICHLOROETHYL)BENZENE	1074119						3.0												
648	XM-CHLORONITROBENZENE	121733						3.0				2.7								
649	*2,4-DICHLORONAPHTHALENE	2198756						3.0												
650	CYCLOPENTENE	142290						3.0										2.2		
651	X+$M-DICHLOROBENZENE	541731						3.0					-0.2							
652	X*+$NITROBENZENE	98953						3.0	-1.4											
653	1-CHLOROTRICYCLO(4.3.1.13.8)UNDECANE	27011467						3.0												
654	DECAMETHYLCYCLOPENTASILOXANE	541026						3.0				1.7								
655	2-CHLORO-1,3,5-TRIMETHYLBENZENE	1667045						3.0												
656	1-CHLORO-2(PHENYLETHYNYL)BENZENE	10271575						3.0												
657	2-METHYLBENZOTRIAZOLE	13351730						3.0												
658	XETHYLENE GLYCOL, BIS(2-CHLOROETHYL) ETHE	112265						3.0					2.8							
659	CYCLODODECANOL	830137						3.0												
660	DIMETHYL SUBERATE	1732098						3.0												
661	METHYL SUCCINATE,DIMETHYL ESTER	1604111						3.0												
662	N-METHYL ETHENAMINE	38239279						3.0												
663	XHEPTANOIC ACID,ETHYL ESTER	106309						3.0												
664	2-(2-CHLOROETHOXY)ETHANOL	628897						3.0												
665	UNDECANOIC ACID,METHYL ESTER	1731868						3.0												
666	XBENZENEACETIC ACID,ETHYL ESTER	101973						3.0							2.9					
667	METHYL P-ETHYLBENZOATE	4346183						3.0												
668	XCLOFIBRATE	637070						3.0												
669	X9H-FLUOREN-9-ONE	486259						3.0									0.2			
670	X1-METHYL-2,4-DINITROBENZENE	121142						3.0	-0.4											
671	2,4-DICHLOROPHENOXY ACETIC ACID, METHYL	54571488						3.0												
672	METHYL ISONONANOATE	2177868						3.0												
673	XETHYL CAPRYLATE	106321						3.0												
674	2-KETOPENTANEDIOIC ACID, DIMETHYL ETHER	13192046						3.0												
675	CLOFIBRIC ACID,METHYL ESTER	55162419						3.0												

(Continued)

TABLE 9. (Continued)

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COMBINED CONCENTRATE REPORT(PART I.A)

	COMMON NAME	CAS NO.	*	VLC	V1X	T2D	T1C	T1K	T1Y	T4C†	T4K†	M2C	N2C	P2C	P2K	O2C	O2K	S2C	S2K	X1C	X1K
				RELATIVE SIZE																	
676	METHYL ISOTRIDECANOATE	1731080							3.0												
677	ETHYL 7-METHYLMYRISTATE	17670756							3.0												
678	METHYL PENTACOSANOATE	55373892							3.0												
679	1-HEXANOL	111273		0.2				3.0													
680	XHEXYL METHYL KETONE	111137			0.0			3.0			0.6*							2.2			
681	2,5-HEXANEDIOL	2935446				1.6	3.0	3.0													
682	5-HEXEN-2-OL	54774275				2.0	2.0	3.0				2.6									
683	XN-AMYL ALCOHOL	71410					3.0	3.0		1.6						1.9		1.2			
684	XNICOTINE	54115					2.0	3.0		-0.4	1.6						1.9		0.2		0.2
685	3-METHYL-4-HEPTANONE	15726155						3.0													
686	2-DODECANOL	10203288						3.0													
687	2-HYDROXY-6-METHYLBENZOIC ACID	567613					3.0									2.9					
688	4-OXO-NONANOIC ACID	6064524					3.0														
689	2-BROMO-1,2-DICHLOROPROPANE	17759885					3.0						2.7								
690	1-BROMO-2,3-DICHLOROPROPANE	33037079					3.0						1.7								
691	1-(1,3-DIMETHYLBUTOXY)-2-PROPANOL	54340895					3.0														
692	TRIPROPYLENE GLYCOL	1638160					3.0														
693	BUTYLBENZYLPHTHALATE	38411120					3.0														
694	X2,6-LUTIDINE	108485					3.0			0.6							-0.1				
695	X2,4-LUTIDINE	108474					3.0			-0.4				0.8							
696	2,3-LUTIDENE	583619					3.0			-0.4											
697	2,4,6-COLLIDINE	108758					3.0									0.9					
698	3,4,4-TRIMETHYL-2-CYCLOHEXEN-1-ONE	17299411					3.0										1.9	2.2			
699	2-PHENYL ACROLEIN	495103					3.0														
700	1-METHYLISOQUINOLINE	1721933					3.0										2.9		0.2		
701	2-3-DIMETHYL QUINOLINE	1721897					3.0										-0.1				
702	X+PHENANTHRENE	85018		-1.0	3.0	1.0	1.0*	2.0*				0.6*	0.7*		2.9*		1.9*	0.2*	1.2*		-0.8
703	XSDICYCLOHEXYL PHTHALATE	84617		3.0	0.0					2.6*	0.6*						2.9*				
704	1,2-DIHYDRO-4-PHENYLNAPHTHALENE	7469401	A		3.0										1.9*		-0.1*				
705	M-DIETHENYLBENZENE	108576	A		3.0	1.0					2.6*						2.9*				-0.8
706	1-PHENYL-3-BUTEN-2-ONE	37442550	A		3.0												1.9*				
707	3-7,11-TRIMETHYL-3-DODECANOL	7278651				3.0															
708	XCETYL ALCOHOL	36653824				3.0				0.6*				0.8*			1.9*	2.2*		2.0	
709	2,2#-BI-1,3-DIOXOLANE	6705891				3.0															
710	N-PROPOXY ETHANOL	2807309				3.0															
711	2-METHYLCYCLOPENTANONE	1120725														1.9*	0.9*			3.0	
712	~~PHOSPHORIC ACID~~	~~456~~																		~~3.0~~	
713	O-ALLYLTOLUENE	1587048	A		1.0	1.0					2.6*				-0.2*	2.9	2.9*				
714	P-ETHYL-ISOPROPYLBENZENE	4218488	A		1.0						0.6*				0.3*	2.9					
715	M-ETHYLISOPROPYLBENZENE	4920994	A		0.0						-0.4*					2.9	-0.1*				
716	(1,1-DIMETHYLPROPYL)BENZENE	2049958	A		1.0						0.6*				1.1*	2.9	0.9*				
717	1-METHYL INDAN	767588			0.0								1.7		0.8*		2.9*		0.2*		
718	1-ETHYL INDAN	4830993	A		-1.0										2.8*		2.9*				
719	1-METHYL-1,2-DIPHENYLETHANE	5814857	A		1.0										2.0*		2.9*				1.2
720	HEXAN-3-ONE	589388								-0.4				2.8	2.8	2.9					2.2

* SEE LAST PAGE OF TABLE

(Continued)

TABLE 9. (Continued)

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COMBINED CONCENTRATE REPORT(PART I.A)

	COMMON NAME	CAS NO.	RELATIVE SIZE																		
			*	V1C	V1X	T2B	T1C	T1X	T1V	T4C†	T4X†	M2C	N2C	P2C	P2X	O2C	O2X	S2C	S2X	X1C	X1X
721	6-METHYL TETRALIN	1688519											1.7		2.0*		2.9*				
722	2,3,4-TRIMETHYLBENZOIC ACID	1076477												1.0		2.9					
723	2-METHYL-2-NONEN-4-ONE	2903233												2.0		2.9					
724	XCHLOROACETIC ACID	79118													1.0	1.9	2.9		2.2		
725	P-DIISOPROPYL BENZENE	100185													1.0	2.9		-0.0			
726	1-HEPTENYLBENZENE	829992													1.0		2.9				
727	2,3,6-TRIMETHYL BENZOIC ACID	2529364														2.9					
728	3-METHYL-2,2-DIOXIDE-1H-2,1,3-BENZOTHIAP	2225403														2.9					
729	XCHLOROACETONE	78955														2.9					
730	ISOPROPYL ACETATE	108214														2.9					
731	.BETA.-OXO-BENZENEACETIC ACID, ETHYL EST	614277														2.9					
732	1,3-DIHYDRO-2,2-DIOXIDE-2,1,3,BENZOTHIAD	1819061														2.9					
733	METHYLISOBUTYL BENZENE	100														2.9					
734	SEC-BUTYL ALCOHOL	78922														2.9	1.9				
735	3,5,5-TRIMETHYL-2(5H)-FURANONE	50598500														2.9					
736	2-PROPYLCYCLOHEXANONE	94655														2.9					
737	~~CHLOROFORM~~	~~67663~~														~~2.9~~	~~1.9~~				
738	5-METHYL-5-PHENYL-2-HEXANONE	14128611														2.9					
739	TETRAMETHYLBENZENE PROPANOIC ACID	55683108														2.9					
740	2,2-DIMETHYLPROPANOIC ACID, 2,4,6-TRIMET	54644405														2.9					
741	6-UNDECANONE	927491														2.9					
742	2,6-DIMETHYLCYCLOHEXANOL	5337724														2.9					
743	HEXAHYDRO-3-(2-PROPENYL)-2H-AZEPIN-2-ONE	29559340															2.9				
744	1(2,6-DIHYDROXY-4-METHOXYPHENYL)ETHANONE	7507493															2.9				
745	XMANDELIC ACID	90642															2.9				
746	(2-CHLORO-2-PROPENYL)OXYBENZENE	53299539															2.9				
747	DECYL VINYL ETHER	765059 A															2.9*				
748	.ALPHA.-HYDROXY-.ALPHA.-METHYL BENZENE A	515388															2.9				
749	4-BUTYL-1,3-CYCLOPENTANEDIONE	54244723															2.9				
750	PHTHIOCOL	483556															2.9				
751	P-ISOBUTYLTOLUENE	5161046															2.9				
752	XORCINOL	504154															2.9				
753	DIBUTYL-3-METHYLGLUTARATE	56051686															2.9				
754	7-METHYL-7-HEPTADECANOL	55723938															2.9				
755	CYCLOHEXYL CHLORIDE	542187		2.0								2.9	1.7					1.2	2.2		
756	1-PHENYLNAPHTHALENE	605027 A		1.0											2.1*		-0.1*				
757	2-PHENYLNAPHTHALENE	612942 A		1.0											2.0*						
758	2-ETHYL TETRALIN	32367547 A		1.0							1.6*				2.0*		1.9*				
759	X2-METHYLANTHRAQUINONE	84540 A		-1.0	1.0										2.0*						
760	4-METHYL INDAN	824226 A		0.0							2.6*				2.1*			0.2			
761	BENZILIDENEACETONE	122576 A													2.0*		1.9*				
762	2,4-DIMETHYL-1-SEC-BUTYLBENZENE	1483609 A									1.6*				2.0*	1.0	1.9*				
763	~~TERPIN~~ SEE NO. 565	~~00535~~									~~0.0~~				~~0.0~~						
764	4-ETHYLBENZYL ALCOHOL	760592 A													2.0*		1.9*				
765	VERATRALDEHYDE	120149													2.0			2.2			

* SEE LAST PAGE OF TABLE

(Continued)

TABLE 9. (Continued)

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COMBINED CONCENTRATE REPORT(PART I.A)

	COMMON NAME	CAS NO.	*	RELATIVE SIZE																	
				V1C	V1X	T2B	T1C	T1X	T1V	T4C	T4N	M2C	N2C	P2C	P2X	O2C	O2X	S2C	S2X	X1C	X1X
766	1,3-DIMETHYNAPHTHALENE	575417	A												2.0*						
767	(2-METHYL-1-PROPENYL) BENZENE	768490	A												2.0*	0.9	1.9*		0.2*		
768	P-DIPROPYLBENZENE	4815570	A												2.0*						
769	(1,1-DIMETHYLBUTYL) BENZENE	1985575	A												2.0*		1.9*				
770	XAZULENE	275514	A												2.0*				1.2		
771	1-METHYLFLUORENE	1730376	A												2.0*						
772	5-METHYL-2-HEXANOL	627598													2.0						
773	3,5,5-TRIMETHYL-2-CYCLOPENTEN-1-ONE	24156954													2.0		0.9				
774	OCTAHYDROINDENE	496106	A												2.0*				0.2*		
775	TRIETHYLENE GLYCOL, DIMETHYL ETHER	112492													2.0						
776	XOO-XYLENE	95476				2.0				0.6				2.0				2.2	2.2		
777	BUTYL FORMATE	592847				2.0								2.0							
778	IODOCYCLOHEXANE	626620										2.6	1.7	2.0		1.0		0.2			
779	2,2-DIMETHYLSUCCINIC ACID	597433												2.0							
780	TRANS-3-BUTYLTETRAHYDRO-2-METHYLFURAN	36712206												2.0							
781	4-HYDROXY-3-METHYL-2-(2-PROPENYL)-2-CYCL	551451												2.0							
782	OCTAHYDRO-4A,8-DIMETHYL-3-ISOPROPYL-2(1H	55332031												2.0							
783	2,4-DIMETHYL-2-PENTANOL	625069												2.0							
784	D-FENCHONE	4695629												2.0				-0.8			
785	1,2-DIMETHYL-3-ISOPROPENYLCYCLOPENTANOL	4899874												2.0							
786	4,8-DIMETHYL-7-NONEN-2-ONE	3664640												2.0				2.2			
787	MENTHONE	10458147												2.0							
788	DICYCLOHEXYLADIPATE	849990												2.0							
789	2-METHYL-1-PENTEN-3-ONE	25044013												2.0							
790	2,2-DIMETHYL-3,5-DECADIENE	55638501												2.0							
791	2,4,6-TRICHLOROANILINE	634935		-1.1			2.0			1.6*			2.7*	1.0*				0.2*	1.2		
792	2,6-DI-T-BUTYL-P-BENZOQUINONE	719222		-1.0	1.0		2.0			1.7*			2.7	1.0*				1.2*			
793	2,4-DICHLOROBENZOIC ACID	50840			2.0			2.0					2.7					2.2			
794	2,4-DIMETHYL HEXANOIC ACID	62329980							1.0				2.7								
795	1-ETHYL-3-METHYL BENZENE	620144							1.0				2.7			1.0					
796	1,6 DIMETHYL-4-ISOPROPYL-NAPHTHALENE	483783								0.6		0.6	2.7	1.0		0.0		0.2			
797	1,2,3-TRIMETHYL BENZENE	526738								-0.4		1.6	2.7	1.0	-0.2			1.2			
798	1-(3,3-DIMETHYLOXIRANYL)ETHANONE	4478631								1.6			2.7					2.2			
799	2,2-DIMETHYL BUTYRIC ACID	595379									1.6		2.7					2.2			
800	2-ETHYLBUTYRIC ACID	88095										1.6	2.7								
801	4,4-DIMETHYL-1,3-DIOXANE	766156											2.7								
802	X3,4-DICHLOROPHENOXYACETIC ACID	588227											2.7								
803	DODECAMETHYLCYCLOHEXASILOXANE	540976											2.7					0.2			
804	X2,6-DIMETHYLNAPHTHALENE	581420											2.7								
805	XO-CHLORONITROBENZENE	88733											2.7								
806	XMESITYLENE	108678											2.7	1.0				0.2	2.2		
807	1-(DICHLOROMETHYL)-4-ETHYLBENZENE	54789296											2.7								
808	1,1-DIBUTOXY-BUTANE	5921802											2.7								
809	CIS-9-OCTADECENAMIDE	301020											2.7								
810	X*TRIPHENYL PHOSPHATE	115866											2.7								

* SEE LAST PAGE OF TABLE

(Continued)

TABLE 9. (Continued)

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COMBINED CONCENTRATE REPORT(PART I.A)

	COMMON NAME	CAS NO.	RELATIVE SIZE																	
			V1G	V1X	T2B	T1G	T1X	T1Y	T4C+	T4X+	N2C	N2C	P2C	P2X	O2C	O2X	S2C	S2X	X1C	X1X
811	3,3,5-TRIMETHYCYCLOHEXANONE	873949										2.7								
812	4-ISOPROPYLACETOPHENONE	645136										2.7					1.2			
813	2-METHYL-3-OXOHEXANOIC ACID, ETHYL ESTER	29304403										2.7								
814	3-OCTANONE	106683										2.7	0.0	0.0			0.2			
815	DIAMYLPHTHALATE	131180										2.7								
816	4,7,7-TRIMETHYLBICYCLO(2.2.1)HEPTAN-2-ON	18292985										2.7								
817	X*O-CHLOROTOLUENE	95498						1.0	-0.4		2.6						-0.0	0.2		
818	1,1,2,3-TETRACHLOROPROPANE	18495302							-0.4*		2.6	1.7*	0.0*				0.2*	2.2	1.0	
819	ETHYL BUTYL KETONE	106354							0.6		2.6					1.0	1.2	1.2		
820	XM-AMINOACETOPHENONE	99036								1.8	2.6									
821	ALPHA-CHLOROPROPIONIC ACID	598787									2.6									
822	2,3-DIMETHYL-2-PENTANOL	4911700									2.6									
823	3-CHLORO-2-METHYL-1-BUTENE	5166358									2.6									
824	2,3-DICHLOROISOBUTANAL	10141227									2.6									
825	1-CHLORO-3-(CHLOROMETHYL)BENZENE	620202									2.6									
826	1,4-DIHYDRO-1-METHYL-4-OXONICOTINONITRIL	767986									2.6									
827	2,4,4-TRIMETHYL-2-PENTENAL	53907612									2.6									
828	1-METHYL-4-ISOPROPYL-1,2-CYCLOHEXANEDIOL	33669768									2.6									
829	X3-METHYL-1-BUTANOL ACETATE	123922									2.6						1.2			
830	TIGALDEHYDE	497030									2.6		1.0				1.2			
831	TRIMETHYLOXIRANE	5076197									2.6						2.2			
832	1-HYDROXY-3-METHYL-2-BUTANONE	36960222									2.6									
833	CIS-2,3-EPOXYHEXANE	6124909									2.6									
834	2,4-DIMETHYLPENTANAL	27944792									2.6						1.2			
835	CYCLOHEXYL ETHER	4645152									2.6									
836	3-ETHYL-2,2-DIMETHYLOXIRANE	1192229									2.6						2.2			
837	4-HYDROXY-3-METHYL-2-BUTANONE	3393644									2.6									
838	TRANS,CIS-4,5-DIETHYL-3,5-OCTADIENE	21293027									2.6									
839	3-HYDROXYBENZALDEHYDE	100834	-1.0							2.6										
840	2,2-DIETHOXYETHANOL	621636	0.0							2.6*										
841	6-ETHYL TETRALIN	22531208	0.0							2.6*				1.0*		1.0*				
842	ALPHA-PICOLINE	109068				2.0			2.6											
843	2-HYDROXY-3,5,5-TRIMETHYL-2-CYCLOHEXENE,	35692989					2.0		1.6	2.6										
844	3,3-DICHLORO-2-PROPENOIC ACID	1561202						2.0		2.6			1.0			1.0				
845	2-PHENYLPROPIONIC ACID	492375							2.6	2.6										
846	BETA,BETA-DIMETHYLPHENYLACETIC ACID	826551							2.6											
847	3-PHENYL PENTANOIC ACID	5669178							2.6											
848	3-HYDROXYCAPRIC ACID	14292263							2.6											
849	$DI-N-PROPYL PHTHALATE	131168							2.6											
850	1-ALLYLNAPHTHALENE	2489863							-0.4	2.6										
851	2-METHYLFURAN	534225							2.6								2.2		2.0	
852	N-PHENYL ACETAMIDE	103844							2.6	2.6										
853	XTRIS-B-CHLOROETHYL PHOSPHATE	115968							2.6											
854	BIS(2-ETHOXYETHYL)ETHER	112367							2.6											
855	N,N-DIMETHYLBENZYLAMINE	103833							2.6	1.6						1.0				

(Continued)

TABLE 9. (Continued)

COMBINED CONCENTRATE REPORT(PART I.A)

	COMMON NAME	CAS NO.	RELATIVE SIZE																	
			VLC	VLK	T2B	T1C	T1K	T1Y	T6C	T6K	H2C	H2K	P2C	P2K	Q2C	Q2K	S2C	S2K	X1C	X1K
856	TETRAETHYLENE GLYCOL DIMETHYLETHER	143248							-0.4	2.6										
857	TETRAPROPYLENE GLYCOL METHYL ETHER	20324349							2.6											
858	4-CHLOROCROTONIC ACID	18197903								2.6				0.0						
859	XSACCHARIN	81072								2.6										
860	M-DI-SEC-BUTYLBENZENE	1079965								2.6										
861	P-DI-SEC-BUTYLBENZENE	1014411								2.6										
862	X2-METHYL-2-PHENYLOXIRANE	2085883								2.6										
863	6,6-DIMETHYL-2,5,10-UNDECANETRIONE	50464965								2.6							2.2			
864	2-METHYL-2-CYCLOPENTEN-1-ONE	1120736								2.6					1.3		2.2	1.2		
865	3,4-DIMETHYLBENZALDEHYDE	5973717								2.6						1.0				
866	3-BROMOHEPTANE	1974056						2.3												
867	N-BENZOYL-L-ALANINE, METHYL ESTER	7244679	1.0														2.2			
868	1-HEPTADECANOL	1454859			2.0												2.2			
869	1,1,2-TRICHLORO-1-PROPENE	21400259				1.0					1.6	1.7						2.2		
870	3-METHYL-2-HEPTANOL	31367461							1.6								2.2			
871	X*O-CHLOROANILINE	95512							-0.4	0.6							2.2			
872	2-ETHYLACETOACETIC ACID	4433056												0.0	1.0		2.2			
873	TRIDECYLIC ACID	638539													1.0		2.2			1.2
874	5-METHYL-3-HEXEN-2-ONE	5166530													1.0		2.2			
875	4,4-DIMETHYLHEXANAL	9932912														0.0	2.2			
876	TETRAHYDRO-2H-PYRAN-2-ONE	542289															2.2			
877	2-DECANOL	1120065															2.2			
878	XP-TERT-BUTYL PHENOL	98544															2.2			
879	2,5-DICHLORO-4-METHYLBENZOIC ACID	21460888															2.2			
880	1-NAPHTHOIC ACID	86555															2.2			
881	2-CHLORO-3-METHYL-2-BUTENE	17773658															2.2			
882	*+$PENTACHLOROBIPHENYL + OTHER PCBS	888															1.2	2.2		
883	2,4-DICHLOROPENTANE	625672															2.2			
884	3,6-DIMETHYL-3-HEPTANOL	1573288															2.2			
885	1-ETHOXY-2-HEPTANONE	51149783															2.2			
886	3-CYCLOHEXYL-4-PENTEN-2-ONE	55702540															2.2			
887	3-METHYL-1,2,4-CYCLOPENTANETRIONE	4505548															2.2			
888	3-ETHOXYPROPANAL	2806851															2.2			
889	1-(1-CYCLOHEPTEN-1-YL)ETHANONE	14377118															2.2			
890	4,4,5,5-TETRAMETHYL-2,7-OCTANEDIONE	17663273															2.2			
891	XBETA-CITRONELLOL	106229															2.2			
892	3-ETHYL-4-METHYL-3-PENTEN-2-ONE	22287112															2.2			
893	4,4-DIMETHYLCYCLOHEXENE	14072867															2.2			
894	1-NITRO-2-OCTANONE	16867819															2.2			
895	~~2,3,3-TRIMETHYLHEXANE~~	16747287															2.2			
896	5,5-DIETHOXY-3-PENTYN-2-ONE	55482845															2.2			
897	3-ALLYL-2,4-PENTANEDIONE	3508785															2.2			
898	2,2-DIMETHYL-3-PROPYLOXIRANE	17612350															2.2			
899	7-METHYL-3-OCTEN-2-ONE	33046818															2.2			
900	MENTHYL ACETATE	16409453															2.2			

(Continued)

TABLE 9. (Continued)

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COMBINED CONCENTRATE REPORT(PART I.A)

	COMMON NAME	CAS NO.	VLC	VLX	T2B	TIC	TIX	TLY	T4C	T4X	NEC	NEG	PDC	PDX	OGC	OGX	SZC	SZK	KIC	KAN
			RELATIVE SIZE																	
901	3-METHYL-3-DECEN-2-ONE	54411039																		
902	6-METHYL-3(2H)-BENZOFURANONE	20895414															2.2			
903	DI-SEC-BUTOXYMETHANE	2568925															2.2			
904	XANTHENE	92831															2.2			
905	6-DODECANOL	6836380															2.2			
906	2-METHYL-2-HEXANOL	625230															2.2			
907	5-METHYL-3-METHYLENE-2-HEXANONE	1187877															2.2			
908	CYCLODECANOL	1502052															2.2			
909	1-(ETHENYLOXY)PENTANE	5363633															2.2			
910	CIS-3,4-DIMETHYL-3-HEXEN-2-ONE	20625454															2.2			
911	PHENYLBUTANAL	10328115															2.2			
912	CIS-5-BUTYLDIHYDRO-4-METHYL-2(3H)-FURANO	95813326															2.2			
913	2,6-DIISOPROPYLPHENOL	2078548															2.2			
914	ALPHA-FARNESAL	4955322															2.2	2.2		
915	3A,4,5,7A-TETRAHYDRO-4-HYDROXY-3A,7A-DIM	94346864															2.2			
916	BUTYL CYANATE	1768247															2.2			
917	ETHYL AMYL KETONE	541855															2.2			
918	3,8-NONADIEN-2-ONE	95282981															2.2			
919	3A,4,7,7A-TETRAHYDRO-2-PROPYL-1H-ISOINDO	2021287															2.2			
920	2-HEXEN-1-OL	249189															2.2			
921	ISOCYANOETHANE	624793															2.2			
922	4-PENTEN-2-OL	625310															2.2			
923	3-CHLORO-3-BUTEN-2-ONE	683705															2.2			
924	[2-(PENTYLOXY)ETHYL]CYCLOHEXANE	54852754															2.2			
925	DIMETHYLSULFONE	67710															2.2			
926	2,4-DI-TERT-BUTYLPHENOL	96764															2.2			
927	2-CHLORO-2-PROPENOIC ACID	598798															2.2			
928	BETA-RESORCYLIC ACID	89861																2.2		
929	XP-NITROBENZOIC ACID	62237																2.2		
930	~~HEPTANE~~	~~142825~~																~~2.2~~		
931	TETRAHYDROFURFURYL ALCOHOL(THFA	97994																2.2		
932	LOLIOLIDE	1133835																2.2		
933	X*+BFLUORANTHENE	206440	-2.1					2.0	-0.4	-0.4	0.4			0.0				2.2		
934	METHYL HEPTADECANOATE	1731936	-1.0					2.0										-0.0		
935	XPROPIOPHENONE	93550		0.0				2.0												
936	(1-NITROETHYL)BENZENE	7214611		1.0				2.0								0.4				
937	2,3,4,5-TETRACHLOROANILINE	634833				1.0		2.0			0.6									
938	XO-CHLOROPHENOL	95578						2.0												
939	2-METHYL-1-NAPHTHALENOL	7469774						2.0												
940	2,3-DICHLOROBUTENE	7581977						2.0												
941	1-BROMO-2-CHLORO-2-BUTENE	94410843						2.0												
942	2,4-DICHLORO-1-(CHLOROMETHYL)BENZENE	94995						2.0												
943	1,2-DICHLORO-4-(CHLOROMETHYL)BENZENE	102476						2.0												
944	X+9H-FLUORENE	86737						2.0												
945	P-BROMOTOLUENE	106387						2.0												

(Continued)

TABLE 9. (Continued)

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COMBINED CONCENTRATE REPORT(PART I.A)

				RELATIVE SIZE																	
	COMMON NAME	CAS NO.	*	V1C	V1X	T2B	T1C	T1X	T1Y	T4C†	T4X†	M2C	N2C	P2C	P2X	O2C	O2X	S2C	S2X	X1C	X1X
946	1,2-DICHLORO-3-NITROBENZENE	3209221							2.0										1.2		
947	2-CHLORO-P-CYMENE	4395793							2.0												
948	2-CHLORO-1-(4-ETHYLPHENYL)-2-METHYL-1-PR	55012696							2.0								-0.1				
949	+X*$LINDANE	58899							2.0				1.7					1.2	0.2		
950	METHYL DICHLOROACETATE	116541							2.0									1.2			
951	XURETHANE (ETHYLCARBAMATE)	51796							2.0		0.6						1.9				
952	4-CHLOROPHENYL ACETIC ACID, METHYL ESTER	34040647							2.0												
953	METHYL ANTEISOPENTADECANOATE	5129668							2.0												
954	P-CHLORO-2-NITROANILINE	89634							2.0												
955	2,4-D,ETHYL ESTER	54571499							2.0												
956	ALPHA-KETOGLUTARIC ACID	328507						2.0													
957	METHYL PROPENYLOXY KETONE	17257793					2.0														
958	4-HYDROXY-4-METHYLCYCLOHEXANONE	17429026					2.0														
959	3,4,5-TRIMETHYL-2-CYCLOPENTEN-1-ONE	55683211					2.0									1.9	1.9				
960	XETHYLENE GLYCOL	107211					2.0														
961	GAMMA-PICOLINE	108894					2.0			-0.4											
962	2,5-LUTIDINE	589935					2.0														
963	2,3,6-TRIMETHYLPYRIDINE	1462846					2.0														
964	5-ETHYL-2-PICOLINE	104905					2.0														
965	2,3,4-TRIMETHYLPYRIDINE	2233296					2.0														
966	2,4,5-COLLIDINE	1122390					2.0														
967	2-ETHYL-6-PICOLINE	1122696					2.0														
968	4,4,5-TRIMETHYL-2-CYCLOHEXEN-1-ONE	17429297					2.0														
969	ISOVALERAMIDE	541468					2.0														
970	XQUINOLINE	91225					2.0														
971	XQUINAIDINE	91634					2.0			0.6											
972	DIPROPYLENE GLYCOL	110985					2.0				0.6										
973	2-(1-METHYL-2-PIPERIDINYL)-PYRIDINE	19730042					2.0														
974	METHYLOCTADEC-10-ENOATE	13038454		0.0		2.0															
975	METHYL-9,11-OCTADECADIENOATE	13038476		1.0		2.0															
976	2-METHYL TETRALIN	3877198	A		2.0										1.0*		0.9*				-0.0
977	3-METHYL INDENE	767602	A		2.0																
978	DIMETHYL NAPHTHALENE	300	A		2.0																
979	3-ETHOXYPROPIONITRILE	2141620			2.0																
980	(2-PHENYLETHYL)ACETATE	103457			2.0																
981	2-XYLYLETHANOL	27577964			2.0																
982	XCINNAMALDEHYDE	104552			2.0						1.6*										
983	ACETYL BIPHENYL	947911			2.0													-0.0			1.2
984	4-OCTANONE	589639			2.0												0.9*				
985	3-BUTEN-2-OL	598323				2.0															
986	B-ETHYLSTYRENE	7564638	A			2.0					1.6*		0.7								
987	1-HEPTADECENE	6765395				2.0															
988	3,5-DIMETHYL-2-CYCLOHEXEN-1-ONE	1123097				2.0					1.6						0.9		0.2		
989	DODECANAMIDE	1120167				2.0											1.9				0.2
990	METHYL-2,3-DIMETHYL BENZOATE	15012369				2.0															

* SEE LAST PAGE OF TABLE

(Continued)

TABLE 9. (Continued)

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COMBINED CONCENTRATE REPORT(PART I.A)

	COMMON NAME	CAS NO.	*	V1C	V1X	T2B	T1C	T1X	T1Y	T4C†	T4X†	M2C	N2C	P2C	P2X	O2C	O2X	S2C	S2X	X1C	X1X
				RELATIVE SIZE																	
991	METHYL-11-OCTADECENOATE	52380333				2.0															
992	METHYL-9,12,15-OCTADECATRIENOATE	301008				2.0															
993	%N,4-DIMETHYLBENZENESULFONAMIDE	640619				2.0															
994	3-METHYL-1-PENTANOL	589355				2.0															
995	%+ACENAPHTHALENE	83329								-0.4								-0.8		2.0	
996	OCTADECANOL	26762447								1.6*										2.0	
997	ANTEISOHEPTADECANOIC ACID	457																		2.0	
998	4-(1,5-DIMETHYL-3-OXOHEXYL)CYCLOHEXANECA	38963916																		2.0	
999	1-(2-PROPENYLOXY)HEPTANE	16519247																		2.0	
1000	8-NONENE-2-ONE	5009325																		2.0	
1001	N-PROPYL-1-HEXANAMINE	20193231		-1.8												1.9*					
1002	PHENYLCYCLOHEXANE	827521	A		1.0						1.6*				1.8*		1.9*				0.2
1003	ETHYLVALERATE	539822			0.0											1.9					
1004	%ETHYL HEXANOATE	123660			0.0											1.9					
1005	1-(1-ETHYLPROPYL)-2-PROPYLBENZENE	54789150	A		-1.0						1.6*				1.9*		1.9*				-0.8
1006	DIETHYL TOLUENE	25550134	A		1.0	1.0							0.7			1.9					
1007	1,6-DIMETHYL DECALIN	1750512				1.0										1.9					
1008	%M-TOLUQUINONE	1125800					1.0										1.9				
1009	4-METHYLCYCLOHEXANE CARBOXYLIC ACID	4331548								0.6						1.9					
1010	PSEUDOCUMENE	95636								-0.4		1.6	1.7	0.8		1.9		1.2			
1011	ACETOACETIC ACID	541504									1.5						1.9				
1012	1,4-DIMETHYL-2-ISOBUTYL BENZENE	55669880	A								-0.4*						1.9*				
1013	2,3,4-TRIMETHYL-2-CYCLOPENTEN-1-ONE	28790865									0.6						1.9				
1014	5-METHYLFURFURAL	620020									0.6					1.9					
1015	1,1-DIMETHYL INDENE	18636550												0.8		1.9		-0.8			
1016	2-PENTENOIC ACID	626982													1.9		1.9				
1017	4-OCTENOIC ACID	18294898														1.9					
1018	%N-UNDECYLIC ACID	112378														1.9					
1019	CLOFIBRIC ACID, M-CHLORO ISOMER	17413739														1.9					
1020	7-OXO-OCTANOIC ACID	14112982														1.9					
1021	1,2,3,3A-TETRAHYDRO AZULENE	33877871														1.9					
1022	~~2,6-DIMETHYLOCTANE~~	~~2051301~~														~~1.9~~					
1023	7-OCTEN-2-ONE	3664606														1.9					
1024	6-METHYL-BICYCLO[4.1.0]HEPTANONE	1484541														1.9					
1025	%FURFURAL	98011														1.9					
1026	6-METHYL-3,5-HEPTADIEN-2-ONE	16647044														1.9					
1027	2-METHYL-2-(1-METHYLPROPYL)-OXIRANE	42328438														1.9					
1028	%DIETHYL SULFITE	623814														1.9					
1029	~~1,2,4-TRIMETHYL-CYCLOHEXANE~~	~~7667552~~														~~1.9~~					
1030	3-ISOPROPYL-2,4-PENTANEDIONE	1540381														1.9					
1031	HEXAHYDRO-4-METHYL-2H-AZEPIN-2-ONE	3623050														1.9					
1032	2-METHLY-5-ISOPROPYLCYCLOHEXANONE	499707														1.9					
1033	2-BUTYL-2-OCTENAL	13019164														1.9					
1034	3,3-DIMETHYL-2(3H)-FURANONE	13524760														1.9					
1035	3-HYDROXY-2,4-PENTANEDIONE,BENZOATE	4620477														1.9					

* SEE LAST PAGE OF TABLE

(Continued)

TABLE 9. (Continued)

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COMBINED CONCENTRATE REPORT(PART I.A)

	COMMON NAME	CAS NO.	*	RELATIVE SIZE																	
			*	V1C	V1X	T2B	T1C	T1X	T1Y	T4C†	T4X†	N2C	N2C	P2C	P2X	O2C	O2X	S2C	S2X	X1C	X1X
1036	2,2-DIMETHYLHEXANEDIOIC ACID, DIMETHYL E	17219215														1.9					
1037	VINYL CHLORIDE	75014															1.9				
1038	XCROTONIC ACID	3724650															1.9				
1039	3-PENTENOIC ACID	5204648															1.9				
1040	XOXALIC ACID	144627															1.9				
1041	7-NONENOIC ACID	1022															1.9				
1042	1-ETHYL-2,3-DIMETHYL BENZENE	933982															1.9				
1043	(1-ETHYL-2-PROPENYL)-BENZENE	19947229															1.9				
1044	2,6-DIMETHYLSTYRENE	2039909															1.9				
1045	BIS(3-METHYLPHENYL)METHANONE	2852688															1.9				
1046	1-ACETYLPIPERIDINE	618428															1.9				1.2
1047	CIS-2,3-DIHYDRO-2-METHYL-1H-INDENE-1,2-D	56508400															1.9				
1048	2,3-DIHYDRO-3,3-DIMETHYL-1H-INDEN-1-OL	38393929															1.9				
1049	5-ETHENYL TETRAHYDRO-.ALPHA.,.ALPHA.,5-T	5989333															1.9		0.2		
1050	1-(1-CYCLOHEXEN-1-YL)ETHANONE	932661															1.9				
1051	M-MENTH-1(7)-ENE (R)-(-)	13837713															1.9				
1052	1,7,DIHYDRO-2-(METHYLAMINO)-6H-PURIN-6ON	10030781															1.9				
1053	1-ALLYLBENZENE	637583															1.9				
1054	2(3H)-BENZOTHIAZOLONE	934349															1.9				
1055	XP-TOLUQUINONE	491350															1.9				
1056	4-METHYLPHENANTHRENE	832644			1.8										1.9*						
1057	3',4'-DIHYDROXYACETOPHENONE	1197097			0.0										1.8*						
1058	TRANS-3-METHYL-3-PENTENOIC ACID	41653934													1.8						
1059	5-ETHYLDIHYDRO-2(3H)-FURANONE	695067													1.8						
1060	O-CRESOTIC ACID	83409													1.8				1.2		
1061	PHLOROL	90006													1.8						
1062	2,3-DIMETHYL TETRALIN	21564921													1.8						
1063	OCTYL BENZENE	2189608													1.8			-0.8			
1064	2,4,5-TRIMETHYLBENZALDEHYDE	5779726													1.8				0.2		
1065	3-METHYLSTILBENE	14064483	a												1.8 *						
1066	BENZIL	134816													1.8						
1067	2-(1-(2-METHOXYETHOXY)ETHOXY)ETHANOL	1017													1.8						
1068	XP-CYMENE (P-ISOPROPYL TOLUENE)	99876					1.8							1.8	-0.2						
1069	1,1,2,3,3-PENTACHLOROPROPANE	15104617								-0.4		1.6	1.7	1.8				0.2	1.2		
1070	XDMF (DIMETHYLFORMAMIDE)	68122										1.6		1.8				1.2			
1071	1,6-DIMETHYLNAPHTHALENE	575439											1.7	1.8		-0.1		-0.8			
1072	5-METHYL TETRALIN	2809645											0.7	1.8	-0.2						
1073	2-PROPYLHEPTANOIC ACID	31080394												1.8							
1074	X3,5-DICHLOROPHENOL	591355												1.8							
1075	O-ISOPROPYLBENZOIC ACID	2438042												1.8							
1076	O-ETHYL TOLUENE	611143												1.8	-0.2			1.2			
1077	1-METHYL-2-CYCLOHEXEN-1-OL	23758272												1.8							
1078	TRI-N-PROPYLENE GLYCOL, METHYL ETHER	13133294												1.8							
1079	4-ETHYLPYRIDINE	536754												1.8							
1080	X1,3,6-TRIMETHYL-2,4(1H,3H)-PYRIMIDINEDIO	13509529												1.8							

* SEE LAST PAGE OF TABLE

(Continued)

TABLE 9. (Continued)

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COMBINED CONCENTRATE REPORT(PART I.A)

RELATIVE SIZE

	COMMON NAME	CAS NO.	*	VIC	VIK	T2B	T1C	T1K	T1V	T4C+	T4K+	M2C	N2C	P2C	P2K	O2C	O2K	S2C	S2K	N1C	N1K
1081	XCAPRALDEHYDE	112312												1.0							
1082	3',4'-DIMETHOXYACETOPHENONE	1131620												1.8				0.2			
1083	X*DIPHENYLAMINE	122394									-0.4		1.7	-0.2				1.8	1.2		
1084	BUTYLATED HYDROXY TOLUENE (BHT)	128370			1.0			1.8		1.7			1.7	0.8							
1085	XPHENYL ETHER	101848								1.6			1.7	0.8							
1086	2-METHYL-3-PENTANONE	565695											1.7								
1087	2-ETHYL PENTANOIC ACID	20225245											1.7								
1088	~~XDECANE~~	~~124185~~											~~1.7~~		~~-0.2~~						
1089	~~UNDECANE~~	~~1120214~~											~~1.7~~								
1090	1-ETHYL-3,5-DIMETHYL BENZENE	934747											1.7	0.8			0.9				
1091	4-ETHYL-1,2-DIMETHYL BENZENE	934805											1.7	0.8					0.2		
1092	ISODURENE	527537											1.7					-0.8			
1093	1,2-DIMETHYL INDAN	17057828											1.7	0.8							
1094	X1,4-DIMETHYLNAPHTHALENE	571584											1.7								
1095	P-CHLORONITROBENZENE	100005											1.7								
1096	2,3,6-TRIMETHYLNAPHTHALENE	829265											1.7	-0.2				-0.8			
1097	1,6,7-TRIMETHYLNAPHTHALENE	2245387											1.7	0.8							
1098	1,4,6-TRIMETHYL NAPHTHALENE	2131422											1.7	-0.2							
1099	5-CHLORO-2-METHYLBENZOFURAN	42180825											1.7								
1100	CIS-1,2,3-TRIMETHYL-4-PROPENYLNAPHTHALEN	26130847											1.7								
1101	CHLOROFLUOROBENZENE	55256172											1.7								
1102	1,1,3-TRICHLORO-2-METHYL-1-PROPENE	31702337											1.7								
1103	PENTACHLOROBENZENE	608935											1.7								
1104	2-T-BUTYL NAPHTHALENE	2876359											1.7								
1105	~~DECYLCYCLOHEXANE~~	~~1795160~~											~~1.7~~								
1106	4-PHENYLBICYCLOHEXYL	20273272											1.7					1.2			
1107	X *+$HEPTACHLOR	76448											1.7								
1108	NITROCYCLOHEXANE	1122607											1.7								
1109	2,6-DIMETHYLCYCLOHEXANONE	2816571											1.7								
1110	METHOXYCYCLOHEXANE	931566										1.6									
1111	3-ETHYLHEXANOIC ACID	41065912										1.6									
1112	P-ETHYL TOLUENE	622968										1.6				-0.1					
1113	ACETOIN	513860										1.6						1.2			
1114	2-METHYL-2-ISOPROPYL-1,3-DIOXOLANE	4405167										1.6									
1115	4-PHENYL PENTANOIC ACID	16433435								1.6											
1116	DIMETHYL ISOPROPYL BENZENE	103								1.6											
1117	4-HYDROXY-4-METHYL-2-PENTANONE	123442								1.6											
1118	1-INDANONE	83330								1.6											
1119	2,2*METHYLENEBIS(6-(1,1-DIMETHYLETHYL)-4	119471								1.6											
1120	DIMETHYL INDAN	615									1.6										
1121	2,4,6-TRIMETHYLBENZALDEHYDE	487683	0								1.6*					0.9*			0.2*		
1122	M-ANISALDEHYDE	591311									1.6										
1123	DIBROMOCYCLOHEXENE	8895									1.6										
1124	META-CYMENE (M-ISOPROPYL TOLUENE)	535773													-0.2			1.2			
1125	2-KETO-3-METHYL VALERIC ACID	1460340																1.2			

* SEE LAST PAGE OF TABLE

(Continued)

TABLE 9. (Continued)

COMBINED CONCENTRATE REPORT(PART I.A)

	COMMON NAME	CAS NO.	VLC	VLX	T2B	T1C	T1X	T1Y	T4C	T4X	M2C	N2C	P2C	P2X	O2C	O2X	S2C	S2X	X1C	X1X
			RELATIVE SIZE																	
1126	5-HEXENOIC ACID	1577226															1.2			
1127	2,6-DIMETHYLHEPTANOIC ACID	60148949															1.2			
1128	3,3-DIMETHYLBUTYNE	917920															1.2			
1129	SEC-ISOAMYL ALCOHOL	598754															1.2			
1130	7-OCTEN-4-OL	53907725															1.2			
1131	2-METHYLCYCLOPENTANOL ACETATE	40991933															1.2			
1132	2,4-DIISOPROPYLPHENOL	2934056															1.2			
1133	ETHYL 4-HYDROXYPHENYLACETATE	17138282															1.2			
1134	DIOCTYL AZELATE	103242															1.2			
1135	TRIETHYLENE GLYCOL, PHENYL ETHER	7204162															1.2			
1136	2-ETHYL-3-PROPYLOXIRANE	53897328															1.2			
1137	DMU (DIMETHYL UREA)	5336243															1.2			
1138	P-(1-ETHYLPROPYL)TOLUENE	22975582															1.2			
1139	2-METHYL-1-DODECANOL	57289266															1.2			
1140	2-METHYLENE-1-BUTANOL ACETATE	55670092															1.2			
1141	TETRAHYDROFURFURYL ACETATE	637649															1.2			
1142	5-METHOXY-2-PENTANONE	17429048															1.2			
1143	5-(ACETYLOXY)-2-PENTANONE	5185977															1.2			
1144	PINACOL	76095															1.2			
1145	1,1-DIMETHOXYCYCLOHEXANE	933404															1.2			
1146	METHYL 3,6-DIHYDRO-4,5-DIMETHYL-2H-PYRAN	24588612															1.2			
1147	5-NONANOL	623938															1.2			
1148	1-TERT-BUTOXY-2-METHYLCYCLOHEXENE	40648268															1.2			
1149	0-ISOPROPYLACETOPHENONE	2142656															1.2			
1150	NONYLPHENOL	25154523															1.2			
1151	%2-FUROIC ACID	88142																1.2		
1152	CROTONYLBENZENE	1560061																1.2		
1153	ALLYLACETONE	109499																1.2		
1154	DIPROPYL CARBINOL	589559																1.2		
1155	%GUAIACOL	90051																1.2		
1156	SPIRODODECANE	181157																1.2		
1157	1-PHENYL-1,2-PROPANEDIONE	579077																1.2		
1158	FARNESOL	3790714																		1.2
1159	1-(BROMOMETHYL)-4-METHYLBENZENE	104814						1.0												
1160	P-CHLOROANISOLE	623121						1.0												
1161	1,2,4,5-TETRACHLOROBENZENE	95943						1.0												
1162	(1-CHLOROETHYL)DIMETHYLBENZENE	54411211						1.0												
1163	2-BROMO-4-METHYL-1-ISOPROPYLBENZENE	4478108						1.0												
1164	1-(CHLOROMETHYL)NAPHTHALENE	86522						1.0												
1165	*$TETRACHLOROBIPHENYL	26914330						1.0												
1166	*$PENTACHLOROBIPHENYL	25429292						1.0												
1167	3-HEXYL BROMIDE	3377875						1.0					0.8							
1168	1,1,2-TRICHLOROPROPANE	598776				1.0											-0.8			
1169	5,8-DIMETHYLQUINOLINE	2623509				1.0														
1170	2,3,5-COLLIDINE	695987				1.0														

(Continued)

TABLE 9. (Continued)

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COMBINED CONCENTRATE REPORT(PART I.A)

	COMMON NAME	CAS NO.	*	V1C	V1X	T2B	T1C	T1X	T1Y	T4C	T4X	M2C	N2C	P2C	P2X	O2C	O2X	S2C	S2X	X1C	X1X
				RELATIVE SIZE																	
1171	4-ETHYL-2,6-DIMETHYL PYRIDINE	36917369					1.0														
1172	3-ETHYL-2,4,5-TRIMETHYL-1H-PYRROLE	528694					1.0														
1173	%2,4-DIMETHYLQUINOLINE	1198374					1.0														
1174	TRIETHYLENE GLYCOL N-BUTYL ETHER	143226		1.0																	
1175	METHYL OLEATE	112629		1.0																	
1176	1,2-BENZISOTHIAZOLE	272162		1.0																	
1177	9,12-OCTADECADIENOIC ACID	60333		1.0																	
1178	4-ETHENYL BENZOIC ACID	1075496	A		1.0																
1179	4-HYDROXYACETOPHENONE	7339879			1.0																
1180	2-HYDROXY DECANOIC ACID	5393817			1.0																
1181	%META-CRESOL	108394			1.0																
1182	1-NAPHTHALENOL	90153			1.0																
1183	DIETHYL PHENOL,(UNKNOWN ISOMER)	26967657			1.0																
1184	METHOXYBENZENE	100663			1.0																
1185	2,2-DIMETHYL-1,1-BIPHENYL	605390	A		1.0																
1186	ALPHA-HYDROXY-ALPHA-PHENYL PHENYL ACETIC	76937			1.0																
1187	1-METHYL ANTHRACENE	610480			1.0																
1188	4-METHYL-3-HEPTANONE	6137117			1.0													-0.8			
1189	METHYL PROPIONATE	554121			1.0																
1190	P-METHYL ACETOPHENONE	122009	a		1.0																
1191	2#,4#,6#-TRIMETHYLACETOPHENONE	1667012	a		1.0																
1192	1-T-BUTYL-3-ETHYL-5-METHYL BENZENE	6630019	A		1.0																
1193	2-ALLYL BENZOATE	583040	a		1.0																
1194	1-METHOXYETHYLBENZENE	4013347	a		1.0																
1195	QUINOXALINE	91190			1.0																
1196	ETHYL MARGARATE	14010232	A		1.0										0.8*						
1197	BENZOPHENONE	119619	a		1.0																
1198	%+PYRENE	129000		0.0		1.0									0.8*						
1199	NEOPENTYL ALCOHOL	75843				1.0															
1200	2-ETHOXYBUTANE	2679870				1.0															
1201	HYDROGENATED ABIETIC ACID	4087696				1.0															
1202	1-ETHYL-METHYLCYCLOPENTANE	16747505				1.0															
1203	%$CUMENE	98828				1.0				-1.4				0.8		0.9					
1204	BENZALDEHYDEOXIME	622322				1.0															
1205	METHYL PALMITOLEATE	1128258				1.0															
1206	6-PHENYL-2-HEXANONE	14171892																		1.0	
1207	4,4,5-TRIMETHYL-1,3-DIOXAN-1-OL	54063148																		1.0	
1208	%ETHYL CAPRATE	110383														0.9					
1209	1,3-DIMETHYL-5-(1-METHYLETHYL)-BENZENE	4706905								-0.4							0.9				
1210	2,4-DIMETHYLISOPROPYLBENZENE	4706892								0.6						0.9					
1211	3-PHENYLPENTANE	1196583	a								-0.4*				0.9*	0.9					
1212	3,5,5-TRIMETHYLCYCLOHEX-3-EN-1-ONE	471012									0.6					0.9	0.9				0.2
1213	$N-PROPYL BENZENE	103651												-0.2		0.9		0.2			
1214	1,3-DIMETHYL INDAN	4175535												-0.2		0.3					
1215	4,4-DIMETHYL-2-PENTENOIC ACID	6945353														0.9					

* SEE LAST PAGE OF TABLE

(Continued)

TABLE 9. (Continued)

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COMBINED CONCENTRATE REPORT(PART I.A)

RELATIVE SIZE

	COMMON NAME	CAS NO.	*	VLC	V1X	T2B	T1C	T1X	T1Y	T4C†	T4X†	H2C	N2C	P2C	P2K	O2C	O2X	S2C	S2X	X1C	X1X
1216	C6-BENZENE	250														0.9					
1217	2-METHYL-2-BUTENAL	1115113														0.9					
1218	3-FUROIC ACID	488937															0.9				
1219	TETRAHYDRO-3,6-DIMETHYL-2H-PYRAN-2-ONE	3720227															0.9				
1220	2,3-DIMETHYL-1,4-HEXADIENE	18669528															0.9				
1221	2-METHYL-CYCLOHEXANEMETHANOL	2105400															0.9				
1222	XMETHYLPHENYL CARBINOL	98851															0.9				
1223	3,4-DIHYDRO-1(2H)-NAPHTHALENONE	529340															0.9				
1224	PENTAMETHYLBENZENE	700129															0.9				
1225	XISOQUINOLINE	119653															0.9				
1226	X+$DDE	72559											0.7		0.9						
1227	2,4-DIMETHYLPENTANOL	600362													0.8						
1228	3,3-DIMETHYLBUTANAMINE	3850304													0.8						
1229	2,7-DIMETHYL TETRALIN	13065071	a												0.8*						
1230	2,4-DIMETHYLHEPTANE	2213232													0.8						
1231	2,6-DIMETHYLHEPTANE	1072055													0.8						
1232	2-(2-METHOXYPROPOXY)-1-PROPANOL (A DIPR	13588288													0.8						
1233	ETHYL BENZOPHENONE	18220901	a												0.9*						
1234	2,4-DICHLOROANILINE	554007								-0.4				0.8							
1235	X3,4-DICHLOROANILINE	95761								-0.4				0.8							
1236	2-IODOPENTANE	637978												0.8							
1237	2-METHYLTHIOPHENE	554143												0.8							
1238	1,1,3-TRICHLORO-1-BUTENE	13279862												0.8							
1239	1-ETHYL-2,4-DIMETHYL BENZENE	874419												0.8							
1240	1,6-DIMETHYL-4-ISOPROPYL TETRALIN	483772												0.8					0.2		
1241	2-ETHYL-1,3-DIMETHYL BENZENE	2870044												0.8							
1242	TRIPROPYLENE GLYCOL, METHYL ETHER (ISOME	25498491												0.8							
1243	2-(METHYLTHIO)BENZOTHIAZOLE	615225												0.8				0.2			
1244	NONANAL	124196												0.8							
1245	INDAN	496117											0.7					0.2			
1246	(3-METHYL-2-BUTENYL)BENZENE	4489843											0.7								
1247	1,4-DIHYDRO-2,5,8-TRIMETHYLNAPHTHALENE	30316199											0.7								
1248	X*+$HEXACHLOROBENZENE	118741											0.7	-0.2							
1249	1-METHYL-4-PROPYLBENZENE	1074551										0.6						-0.8			
1250	3,3,3-TRICHLORO-2-METHYLPROPENE	4749273										0.6						-0.8			
1251	COTININE	486566								0.6											
1252	CYCLOHEPTANONE	502421									0.6										
1253	BENZYLAMINE	8894									0.6										
1254	2-METHYL-2,4-PENTANEDIOL	107415									0.6										
1255	X*P-CRESOL	106445		0.2	0.0					-0.4	-0.4*										
1256	1,6-DICHLORO-1,5-CYCLOOCTADIENE	29480420												-0.2					0.2		
1257	4,7-DIMETHYL INDAN	6682719																0.2			
1258	1,5,8-TRIMETHYL TETRALIN	21693516																0.2			
1259	BIS(CHLOROPHENYL)METHANE	25249392																0.2			
1260	DURENE	95932																0.2			

* SEE LAST PAGE OF TABLE

(Continued)

TABLE 9. (Continued)

COMBINED CONCENTRATE REPORT(PART I.A)

	COMMON NAME	CAS NO.	VIC	VIX	T2B	T1C	T1K	T1Y	T4C	T4K	M2C	M2C	P2C	P2K	O2C	O2K	S2C	S2K	X1C	X1K
			RELATIVE SIZE																	
1261	CIS-4-PHENYLBICYCLOHEXYL	21484127																		
1262	4-METHYLENECYCLOHEXANEMETHANOL	1084246															0.2			
1263	2,6,6-TRIMETHYL-BICYCLO(3.1.1)HEPTAN-3-O	547604															0.2			
1264	3-BUTYL-1,2,4-CYCLOPENTANETRIONE	46005098															0.2			
1265	%STYRENE GLYCOL	93561															0.2			
1266	2-METHYL-5-UNDECANONE	50639026															0.2			
1267	(3,3-DIMETHYLCYCLOHEXYLIDENE)ACETALDEHYD	26532241															0.2			
1268	P-(1,1,3,3-TETRAMETHYLBUTYL)PHENOL	140669															0.2			
1269	1,2,3,4-TETRAMETHYL BENZENE	488233															-0.8	0.2		
1270	1-ETHYL-1-METHYL INDAN	56298750																0.2		
1271	1-CHLOROTETRADECANE	2425549																0.2		
1272	1,1-DIPHENYLCYCLOHEXANE	21113553																0.2		
1273	BICYCLO(2.2.2)OCTANE-1,4-DIOL, MONOACETA	54774946																0.2		
1274	4-METHYL BIPHENYL	644386																0.2		
1275	ARACHIDYL ALCOHOL	629969																		0.2
1276	2-METHOXY-1-PROPANOL	1589475	0.0																	0.2
1277	ISOMYRISTIC ACID	543	0.0																	
1278	ISOPENTADECANOIC ACID	544	0.0																	
1279	ABIETIC ACID	624	0.0																	
1280	DIDEHYDROGENATED ABIETIC ACID	625	0.0																	
1281	P-PHENYLACETOPHENONE	496	0.0																	
1282	M-METHOXYPHENYL ACETATE	1024		0.0																
1283	METHYL 3-HYDROXYPHENYLACETATE	42058593		0.0																
1284	%2-METHYL ANTHRACENE	613127		0.0																
1285	2-(PHENYLMETHYL) NAPHTHALENE	613592		0.0																
1286	PHENYL P-PYRIDYL KETONE	56771507		0.0																
1287	7-ETHYLQUINOLINE	7661474		0.0																
1288	DODECYL PHENOL	27193868		0.0																
1289	DIMETHYL ETHYL BENZENE	200																		
1290	1-PHENYL-2-CYCLOPENTEN-1-OL	56667108													-0.1					
1291	O-TOLUALDEHYDE	529204														-0.1				
1292	2,3-BIS(METHYLENE)-BICYCLO(3.2.1)OCTANE	49826542														-0.1				
1293	2,2-DIMETHYLHEPTANE	1071267												-0.2						
1294	*2-METHYL STYRENE	611154												-0.2						
1295	1-IODOPENTANE	620171							-0.4				-0.2				-0.8			
1296	2-ETHYL-1,4-DIMETHYL BENZENE	1758889											-0.2							
1297	%INDENE	95136											-0.2				-0.8			
1298	1,2-DIMETHYL INDENE	53204572											-0.2							
1299	4,7-DIMETHYLBENZOFURAN	28715266											-0.2							
1300	1,2-DIHYDRO-1,5,8-TRIMETHYLNAPHTHALENE	4506369											-0.2							
1301	%*+$2-CHLORONAPHTHALENE	91587											-0.2							
1302	1,3,6-TRIMETHYLNAPHTHALENE	3031081											-0.2							
1303	1,2,8-TRIMETHYLNAPHTHALENE (3,4,5-TR	3876979											-0.2							
1304	1-ETHYL-3-METHYLCYCLOPENTANE	3726474											-0.2							
1305	%+*2,4-DIMETHYLPHENOL (XYLENOL)	105679							-0.4	-0.4			-0.2							

(Continued)

TABLE 9. (Continued)

COMBINED CONCENTRATE REPORT(PART I.A)

	COMMON NAME	CAS NO.	*	V1C	V1X	T2B	T1C	T1X	T1V	T4C†	T4X†	M2C	M2C	P2C	P2X	O2C	O2X	S2C	S2X	X1C	X1X
									RELATIVE SIZE												
1306	DIMETHYL ISOPROPYL BENZENE	105								-0.4											
1307	COUMARONE	271896								-0.4											
1308	4,6-DIISOPROPYL-M-XYLENE	5186685								-0.4											
1309	7-METHYLBENZOFURAN	8898								-0.4											
1310	TRICHLOROHEPTAFLUOROBUTANE	28984807								-0.4											
1311	DIMETHYL ISOPROPYL BENZENE	104								-0.4											
1312	1,2,3-TRIETHYLBENZENE	42205083									-0.4										
1313	XBENZYL CHLORIDE	100447								-1.4											
1314	4-METHYLSTYRENE	766972																-0.8			
1315	2-PHENYLHEXANE	6031023																-0.8			
1316	1,4,6-TRIMETHYL TETRALIN	22824324																-0.8			
1317	4-ISOPROPYL-ALPHA-METHYL STYRENE	2388149																-0.8			
1318	M-TERPHENYL	92068																-0.8			
1319	DECAHYDRO-1,4A-DIMETHYL-7-(1-METHYLETHYL	15404634																-0.8			
1320	1-CHLORO-4-(1-CHLOROETHENYL)CYCLOHEXENE	13547063																-0.8			
1321	2,4,6-TRIMETHYLBIPHENYL	3976350																-0.8			
1322	4-PHENYLBICYCLOHEXYL	20273272																-0.8			
1323	2,4,5,7-TETRAMETHYLPHENANTHRENE	7396385																-0.8			
1324	(1,1#-BICYCLOPENTYL)-2-ONE	4884246																-0.8			
1325	O-TERT-BUTYLPHENOL	88186																-0.8			
1326	P-(1-ETHYL-1-METHYLHEXYL)PHENOL (A NONY	52427131																-0.8			
1327	P-(2,2,3,3-TETRAMETHYLBUTYL)PHENOL	54932784																-0.8			
1328	ETHYL NONADECANOATE	18281044	A															-0.8			
1329	5-DECANONE	820291																	-0.8*		
1330	ISOPALMITIC ACID	545		-1.0																	-0.8
1331	DIBROMOPHENOL	546		-1.0																	
1332	2-(4-METHYL-3-CYCLOHEXENYL)ISOPROPANOL	10482561		-1.0																	
1333	1,2-CYCLOHEXANEDIOL	931179		-1.0																	
1334	BUTYL THIAZOLE	6086222		-1.0																	
1335	2-HYDROXY-5-ISOPROPYL-2,4,6-CYCLOHEPTATR	672764			-1.0																
1336	ACETALDEHYDE DIETHYL ACETAL	105577			-1.0																
1337	7-METHYL-3(2H)-BENZOFURANONE	669845			-1.0																
1338	0-NITROTOLUENE	88722								-1.4											

* THE DESIGNATION A AND a DENOTE A COMPOUND THAT IS A PROBABLE OR POSSIBLE ARTIFACT DUE TO XAD-2 RESIN BLEED. RS ENTRIES LABELED WITH AN ASTERISK ARE PROBABLY ATTRIBUTABLE TO THE BLANK ASSOCIATED WITH CONCENTRATE GENERATION. SEE DISCUSSION IN TEXT OF VOLUME 1.

† ADD 0.3 TO ALL RS VALUES SHOWN FOR T4C AND T4X TO GET THE CORRECT RS VALUE. SEE DISCUSSION IN TEXT OF VOLUME 1 COVERING THESE TWO CONCENTRATES.

TABLE 10. COMBINED LISTING OF IDENTIFIED COMPOUNDS FOUND IN AWT CONCENTRATES

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COMBINED CONCENTRATE REPORT(PART I.A)

	COMMON NAME	CAS NO.	RELATIVE SIZE																	
			V1C	X1C	L2P	L2M	L2N	L2D	C3C	C1P	C1M	C1N	C2N	R1C	R2C	E1C	D2N	B2C	B1M	B1N
1	CLOFIBRIC ACID †	882097			3.0	7.0	7.0	8.0		2.0	6.0	7.0	7.0			4.0	3.0	3.0	3.0	
2	DIOCTYL SEBACATE	122623			4.0					9.1	6.0						3.0		6.0	
3	X+$DI-N-BUTYLPHTHALATE	84742	2.0		9.0	6.0*	7.0	5.0*	9.1			3.0*	3.6*	8.1	7.1	7.0	5.0*	8.1	6.0*	5.0*
4	2-(2-BUTOXYETHOXY)ETHANOL (A DIETHYLE	112345						6.0	9.0	6.0	5.0			6.0	5.0	6.0		9.0	1.0	
5	DIETHYLENE GLYCOL, 4-METHOXYBUTYL BUTYL	1002							9.0											
6	DIETHYLENE GLYCOL, 2-METHOXYBUTYL BUTYL	1003							9.0											
7	X*DIPHENYLAMINE	122394			9.2	1.6			1.0	8.0	3.1	2.0								
8	X+$DIOCTYLPHTHALATE	117840			6.0						6.0			6.0	7.0			2.0		
9	2-ETHYLHEXANOIC ACID	149575	-1.0		4.0	4.0	3.0*	8.0	5.0	3.0*	6.0	2.0*	5.0	6.0	9.0		4.0	4.0	4.0	
10	XBENZOIC ACID	65850		1.0	5.0	5.0	6.0	8.0	2.0*	3.0*	6.0	5.0	5.0	9.0	9.0	9.0	5.0	9.0	5.0	9.0
11	1-(2-BUTOXYETHOXY) ETHANOL	54446785			6.0	3.0			8.0	1.0	3.0	2.0		5.0	9.0	9.1				
12	2,4-DIMETHYLBENZOIC ACID	611018				2.0	4.0	8.0	2.0		4.0	2.0			3.0					
13	XTRIS-B-CHLOROETHYL PHOSPHATE	115964				3.0		5.0		6.0	8.0	4.0	5.0		9.0		3.0		3.1	9.0
14	PHENOXY ACETIC ACID	122598					6.0	8.0				5.0	9.0							
15	M-TOLUIC ACID	99047						8.0						4.0	4.0	2.0	2.0	3.0		
16	2-PHENYLPROPIONIC ACID	492375						8.0					5.0		4.0		2.0			
17	2-ETHYL-3-METHYLMALEIC ACID	41656095						8.0			9.0	3.0			5.0		4.0	4.0	6.0	5.0
18	TRIPROPYLENE GLYCOL, METHYL ETHER	480			4.0	6.1	7.0	6.0			5.3	4.0	2.6	9.0					5.0	4.0
19	TRIPROPYLENE GLYCOL, METHYL ETHER	402			4.0	6.1	7.0	6.0			6.0	3.0							5.0	
20	TRIPROPYLENE GLYCOL, METHYL ETHER	403			4.0	6.1	7.0	6.0											5.0	5.0
21	TRIPROPYLENE GLYCOL, METHYL ETHER	401			3.0	6.1	7.0	6.0			9.2	4.0	4.1	9.0	6.0				5.0	2.0
22	X1-BUTANOL	71363				5.0		7.0			2.0			6.0	6.2	4.0	9.1	6.2		4.2
23	TRIETHYLENE GLYCOL N-BUTYL ETHER	143226	1.0			5.0*			7.0					4.0*						
24	DIOCTYL ADIPATE	123795	0.0	3.6	5.0*	3.0*					4.0*				7.0	4.0*		7.0		
25	XBIS(2-ETHYLHEXYL) ADIPATE	103231	0.0			2.0*		5.0		5.0	5.0	3.0*		7.0					5.0	
26	X$1,1,2,2-TETRACHLOROETHANE	79345		5.0		3.0*			3.0*		7.0*	6.0*	6.0*		6.0*			4.0*	0.0*	
27	XMONOBUTYL PHTHALATE	131704		2.0				7.0		3.0				6.0	6.0	3.0	5.0	5.0	3.0	
28	XPALMITIC ACID	57103		5.0	3.0*	5.0*	6.0*				5.0*		5.0*	6.1*	7.0*			5.0*	5.0*	5.0*
29	XSTEARIC ACID	57114		5.0		5.0*					4.0*			6.0*	7.0*		3.0*	4.0*	4.0*	5.0*
30	ORTHO-TOLUIC ACID	118901			5.0	4.0		7.0	3.0			5.0	5.0	3.0	4.0	2.0	1.0	2.0		
31	4-PHENYL PENTANOIC ACID	16433435			3.0	2.0		7.0												
32	3,3-DIMETHYLBUTYRIC ACID	1070833			3.0	5.0		7.0					4.0							2.0
33	XCAPRYLIC ACID	124072			4.0	3.0	3.0	7.0		3.0	5.0		9.0	6.0	6.0		4.0	3.0	3.0	2.0
34	BUTYLATED HYDROXY TOLUENE (BHT)	128370			4.1			2.0		7.0	3.0	1.0		2.0	1.0		1.2			1.0
35	2,6-DI-TERT-BUTYLPHENOL	128392			5.0					7.0										
36	XPHENYLACETIC ACID	103822				4.0	4.0	7.0						3.0	4.0		2.0	9.0	9.0	9.0
37	3,5-DIMETHYLBENZOIC ACID	499069				2.0	4.0	7.0	3.0		3.0	3.0	4.0	2.0	3.0		2.0			
38	3-PHENYL PENTANOIC ACID	9669170				4.0		7.0				3.0					2.0			
39	XETHOSUXIMIDE	77670				6.0		7.0							4.0		4.0	4.0	9.0	4.0
40	DIETHYLENE GLYCOL, BUTYL ETHER	431				2.0						4.0	4.0		7.0					
41	$BUTYL-BUTOXY ETHYL PHTHALATE	33374286				7.0											2.0			
42	2,5-DIMETHYLBENZOIC ACID	610720					3.0	7.0	2.0			4.0	5.0	2.0				4.0		
43	P-TOLUIC ACID	99945					4.0	7.0			4.0		4.0	3.0	4.0	1.0	2.0	3.0		
44	XP-CHLOROBENZOIC ACID	74113					4.0	7.0	4.0			3.0				2.0	4.0			
45	XSACCHARIN	81072					5.0	7.0				9.0	9.0							2.0

† THIS ENTRY APPEARS OUT OF ORDER. IT SHOULD APPEAR BETWEEN ENTRIES NO. 6 AND NO. 10.

(Continued)

TABLE 10. (Continued)

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                                                                                            EPA 18 CONCENTRATES PAGE 2
                                           COMBINED CONCENTRATE REPORT(PART I.A)
    COMMON NAME                                        CAS NO.                         RELATIVE SIZE
                                                            VIC XIC L2P L2M L2N L2O C1C C1P C1M D1N D2N R1C R2C E1C DEN B2C B1M B1N
46  4-METHYLHEXANOIC ACID                          1961111                      7.0
47  6-NONENOIC ACID                               31502239                      7.0
48  3-ETHYLBENZOIC ACID                           28134318                      7.0
49  BETA,BETA-DIMETHYLBENZENEPROPIONIC ACID        1010406                      7.0
50  2,3-DIMETHYLMALEIC ACID                         488211                      7.0             5.0         4.0     4.0 4.0 5.0
51  1-PHENYLBUTYRIC ACID                           1821121                      7.0 2.0
52  %MANDELIC ACID                                   90642                      7.0
53  O-CHLOROBENZOIC ACID                            118912                      7.0 4.0         5.0 6.0             2.0 2.0
54  3,4-DICHLOROBENZOIC ACID                         51445                      7.0             6.0                 3.0 2.0
55  2-BENZYLACRYLIC ACID                           2495394                      7.0
56  4-(1,5-DIMETHYL-3-OXOHEXYL)-1-CYCLOHEXEN      17844074                      7.0         4.0                 2.0     4.0
57  $BUTYL METHYL PHTHALATE                       34006763                          4.0 3.0         7.0 4.0 4.0 3.0 1.0 4.0
58  TRIETHYLENE GLYCOL, TERT-BUTYL ETHER          29681207                          7.0
59  DIHEXYLADIPATE                                  110388
60  DIISOOCTYLPHTHALATE                           27554263                                              7.0 7.0                 9.0
                                                                                                            7.0
61  DIPROPYLENE GLYCOL, METHYL ETHER                   425              4.6 6.0 6.3         5.2 2.0 3.0
62  2,5-DI-T-AMYL QUINONE                          4584638          2.0                 6.2 3.0 1.0                         9.0 1.0
63  DIPROPYLENE GLYCOL, METHYL ETHER                   426              4.6 6.0 6.1         3.0     2.0 3.0                 4.0 2.0
64  TRIPROPYLENE GLYCOL, METHYL ETHER                  484              6.1
65  %METHYL BUTYLKETONE                             591786      4.0 2.0*6.0*                2.0*                                6.1
66  TRIPROPYLENE GLYCOL, METHYL ETHER             20324338              5.1 1.0
67  TRIPROPYLENE GLYCOL, METHYL ETHER                  486                                              2.0 6.0
68  TRIPROPYLENE GLYCOL; METHYL ETHER                  ...                                                  5.0                 5.0
69  %+$DIETHYL PHTHALATE                               405                                                  6.0                 5.0
70  2-BUTYL-N-BUTYRATE                               84662  0.0 1.0     3.0*                        2.0*5.0 6.0 3.0*    6.0
71  %CAPROIC ACID                                   619976                          6.0
72  %CAPRIC ACID                                    142621  -1.0    4.0 4.0 4.0 6.0     3.0*        4.0 5.0 5.0 3.0*5.0 3.0*5.0 3.0*
73  %MYRISTIC ACID                                  334485  0.0     4.0*4.0*            3.0*6.0         6.0 6.0 1.0*3.0*4.0*
74  PENTADECANOIC ACID                              544638  1.0 4.0 4.0*3.0*            3.0*4.0*    6.0*6.0*6.0*        5.0*4.0*5.0*
75  ELAIDIC ACID                                   1002842  1.0 2.0     3.0*                3.0*        5.0*6.0         3.0*3.0*4.0*
76  DEHYDROABIETIC ACID                             112798  2.0         4.0*    5.0*                        6.0*
77  %+PHENANTHRENE                                 5155704  1.0 1.0 4.0*4.0*6.0         5.0*2.0*        5.0*5.0*2.0*3.0*4.0*3.0*
78  P-PHENYLACETOPHENONE                             85018  -1.0    2.0     1.0*0.0*    6.0 2.0*2.0*    2.0*3.0*    3.0*    1.0*
79  PALMITOLEIC ACID                                   496  0.0                                             6.0 3.0*    4.0*
80  METHYL OLEATE                                  2091294  1.0                                 4.0*        6.0
81  %$DI-ISOBUTYLPHTHALATE                          112629  1.0     6.0
82  %$DICYCLOHEXYL PHTHALATE                         84695  0.0     5.0     4.0*    6.0         2.0*3.0*5.1 6.0 3.0*    5.0
83  %+$BIS(2-ETHYLHEXYL) PHTHALATE                   84617  3.0                     2.6*                        6.0     5.0*    5.0*
84  %LAURIC ACID                                    117817  2.6         2.0*            6.0*        1.0*6.0*    2.0*3.0*    5.0*
85  4-(1,5-DIMETHYL-3-OXOHEXYL)CYCLOHEXANECA        143077      3.0 4.0*3.0*    5.0*        5.0*            6.0     3.0*5.0*3.0*3.0*
86  2-ETHYLBUTANAL                                38963916      2.0             6.0         5.0             4.0*
87  2-METHYL-3-HEXANOL                               97961      6.0
88  %PELARGONIC ACID                                617298      6.0
89  P-T-BUTYLPHENOXY ACETIC ACID                    112050          4.0 3.0 3.0             5.0 2.0 5.0 6.0 6.0     4.0 4.0     2.0
90  8-NONENOIC ACID                                1790045          4.0 4.0 3.0 9.0     5.0 6.0 5.0 9.0
                                                  31642678          3.0 2.0     6.0
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(Continued)

TABLE 10. (Continued)

EPA 18 CONCENTRATES PAGE 3

COMBINED CONCENTRATE REPORT(PART I.A)

	COMMON NAME	CAS NO.	RELATIVE SIZE																	
			V1C	X1C	L2P	L2M	L2N	L2D	C3C	C1P	G1M	G1N	G2N	R1C	R2C	E1C	D2M	B2C	B1M	B1N
91	SUBERIC ACID	505486			2.0								6.0	2.0	4.0		2.0	2.0		
92	X+NAPHTHALENE	91203			1.0		4.0			6.0	6.0					1.0	1.0			
93	9,10-DIHYDRO-9,9-DIMETHYL ACRIDINE	6267023			4.0					6.0										
94	$N-BUTYL-ISOBUTYLPHTHALATE	17851535			5.0		6.0				3.0				6.0	3.0		6.0		
95	ACETYL BIPHENYL	947911			6.0															
96	4-ETHOXYBUTYL BUTANOATE	33931689			6.0				5.0											
97	$METHYL ETHYL PHTHALATE	34006774			5.0						6.0									
98	2-BUTOXYETHYL BUTANOATE	20442062			6.0															
99	XMETHYL PROPYL KETONE	107879			2.0					5.0		6.0								
100	2-PHENYLBUTYRIC ACID	98277				4.0	3.0	6.0	3.0			5.0	5.0		3.0					
101	XPHENOBARBITAL	50066				6.0		6.0			5.0	4.0			3.0	2.0				
102	2,2-DIMETHYL BUTYRIC ACID	595379				3.0		6.0			2.0	4.0				3.0				2.0
103	1-METHOXY-2-PROPANOL	107982				6.0				6.0							5.0		5.0	
104	2-METHYL-3-HEXENOIC ACID	62243576				2.0	3.0	6.0					5.0							
105	2-ETHYLSUBERIC ACID	3971333				6.0					4.0	4.0								
106	ISOVALERIC ACID	503742				4.0	5.0	6.0										4.0	4.0	4.0
107	3-ETHYLHEXANOIC ACID	41065912				5.0									6.0					
108	XAMOBARBITAL	57432				4.0		6.0			4.0								3.0	
109	3,4-DIMETHYLBENZOIC ACID	619045				2.0		6.0						5.0						
110	XSALICYLIC ACID	69727					4.0			2.0		5.0			6.0	3.0	2.0		4.0	5.0
111	XPHTHALIC ACID	88993					3.0							6.0	6.0		3.0	5.0	3.0	2.0
112	2-KETOISOCAPROIC ACID	816660					3.0				6.0									
113	2-METHYLHEPTANOIC ACID	1188029					5.0	6.0												
114	TRIPROPYLENE GLYCOL	1638160					6.0								3.0					
115	P-ISOPROPYL BENZOIC ACID	536663					3.0	6.0	2.0								2.0	2.0		
116	DIPROPYLENE GLYCOL, 2-PROPENYL ETHER	55956257					6.0								3.0					
117	BUTYL BUTYRATE	109217					2.0			3.0					5.0					
118	TRIPROPYLENE GLYCOL, METHYL ETHER (ISOME	25498491					2.0							5.0					6.0	
119	2,2-DIMETHYLVALERIC ACID	1185393						6.0					5.0							
120	XN-HEPTANOIC ACID	111148						5.0			2.0	3.0	3.0	6.0	6.0		4.0	2.0		2.0
121	4-METHYL-4-NITROPENTANOIC ACID	23102025						6.0												
122	4,5-DIMETHYLCYCLOOCTANE CARBOXYLIC ACID	5079						6.0												
123	M-CHLOROBENZOIC ACID	535808						6.0				3.0		3.0	4.0		1.0			
124	2,3-DIMETHYLBENZOIC ACID	603792						6.0				5.0								
125	2,4,5-TRIMETHYLBENZOIC ACID	528985						5.0				4.0	5.0	1.0			1.0			
126	3-HYDROXYCAPRIC ACID	14292263						6.0												
127	X2-NAPHTHOIC ACID	93094						6.0											3.0	
128	CIS-OCTAHYDRONAPHTHALENE CARBOXYLIC ACID	3021736						6.0												
129	5,5-DIMETHYLDIHYDROFURANONE	3123975						3.0			6.0								3.0	4.0
130	3,5-DIMETHYLDIHYDROFURANONE	5145017						3.0			6.0								1.0	3.0
131	N-BUTYLBENZENESULFONAMIDE	3622842							6.0		5.0			4.0				3.0	5.0	
132	3,5-DIMETHYL STYRENE	5379204								3.0	6.0		1.0							
133	XP-TOLUENESULFONAMIDE	70553								6.0		4.0								
134	P-TERT-BUTYLPHENOXYMETHYL ACETATE	54889984								5.0	6.0						2.0			
135	1,2,4-TRIBUTYLBENZENE	14888169								6.0										

(Continued)

TABLE 10. (Continued)

EPA 18 CONCENTRATES PAGE 4

COMBINED CONCENTRATE REPORT(PART I.A)

	COMMON NAME	CAS NO.	RELATIVE SIZE																	
			V1C	K1C	L2P	L2M	L2N	L2O	C3C	C1P	G1M	G1N	G2N	R1C	R2C	E1C	D2N	B2C	B1M	B1N
136	4-TERPINEOL ISOMER	526								6.0										
137	N,N-DIMETHYLHEPTANAMIDE	1115964								6.0	5.0									
138	METHYL ELIADATE	1937628								6.0										
139	METHYLTRIDECYLOCTANOATE	55193798								6.0										
140	BUTYL METHOXYBUTYRATE	1018									6.0									
~~141~~	~~2-METHYLHEPTANE~~	~~592278~~									~~6.0~~									
142	2,4-DICHLOROBENZOIC ACID	50840										6.0							4.0	3.0
143	%OLEIC ACID	112801												4.0	6.0				5.0	6.0
144	3,7-DIMETHYL-6-OCTENOIC ACID	2006												3.0	6.0					
145	TRIS(CHLOROPROPYL)PHOSPHATE	995													6.0					
146	TETRAHYDRO-2-METHYL-2-FURANOL	7326467																6.0		
147	2-METHYL-2,4-PENTANEDIOL	107415																	5.4	3.2
148	2-BUTOXYETHANOL	111762				3.0	1.0	1.0			9.3	3.0	5.0		5.1	4.0	1.0		4.0	3.0
~~149~~	~~%DECANE~~	~~124185~~									~~5.0~~		~~5.0~~				~~4.0~~			
150	HEXAN-3-ONE	589388				5.1					6.0	6.0								
151	4-ISOPROPYLACETOPHENONE	645136			9.1															
152	6-METHYL-5-HEPTEN-2-ONE	110930					2.0												5.1	2.0
153	2,5-HEXANEDIOL	2935446										1.0				5.1		2.0		
154	TETRAHYDRO-1,1-DIOXIDE THIOPHENE	126330												4.2	5.1					
155	BENZOTHIAZOLE	95169	1.0		3.0*	3.0*	5.0*	5.0*		5.0*	5.0*	5.0*	5.0*	3.0*			2.0*			
156	DIPROPYLENE GLYCOL METHYL ETHER (1-(2-	13429077			3.0	3.0	4.0	9.0												
157	ADIPIC ACID, DIHEXYL ESTER	110338						4.0						3.0	9.0					
158	X+$BUTYL BENZYL PHTHALATE	85687							5.0	1.0	4.0		2.0					5.0		
159	2,6-BIS(1,1-DIMETHYLETHYL)-4-ETHYLPHENOL	4130421			5.0						4.0									
160	%BENZALDEHYDE	100527			3.0	1.0	1.0	1.0			4.0	9.0	2.0		1.0	3.0	1.0		2.0	1.0
161	ISOPENTADECANOIC ACID	544													9.0		3.0			
162	X*+$PENTACHLOROPHENOL	87865	0.0		5.0			1.0*		4.0*	4.0*	4.0*	5.0		1.0*	1.0*		1.0*	1.0*	1.0*
163	X*+$2,4,6-TRICHLOROPHENOL	88062	-2.0					1.0*	5.0	3.0		2.0*	6.0	2.0	4.0			1.0*		
164	X+PYRENE	129000	0.0		3.0					3.0	1.0*									
165	%TRIBUTYL PHOSPHATE	126738	1.0	2.0	4.0*									4.0*	5.0*	1.0*		5.0*		
166	METHYL PALMITATE	112390	2.0							5.0*					2.0*			2.0*		
167	METHYL STEARATE	112618	1.0		5.0*			0.0*		5.0*										
168	2-ETHYL-1-HEXANOL	104767	-1.0		4.0			1.0*		5.0	3.0*	2.0*		3.0*	4.0			3.2*	3.6	
169	2,6-DI-T-BUTYL-P-BENZOQUINONE	719222	-1.0		2.0*	2.0*			2.0*	9.0	4.0	2.0*		3.0*			1.0*	2.0*	2.0*	
~~170~~	~~CARBONIC ACID~~	~~463~~		~~5.0~~																
171	%1,4-DIOXANE	123911		4.0							2.0*		9.0*	3.0*						2.0*
172	$ETHYLBENZENE	100414		4.0	5.0*	2.0*		0.0*					1.0*						1.0*	
173	%$P-XYLENE	106423		4.0	5.0*	2.0*		0.0*									1.0*			
174	%AZELAIC ACID	123999		2.0									5.0	4.0*	5.0		3.0*	4.0*	3.0*	
175	ANTEISOHEPTADECANOIC ACID	457		2.0											5.0					
176	MARGARIC ACID	506127		3.0										4.0*	5.0*		2.0*	3.0*		4.0*
177	4-METHYL-2-PENTANOL	108112		1.0		5.0			2.0*						1.0*			4.0		
178	2-HEXANOL	626937		1.0	2.0*	5.0														
179	3-METHYLCYCLOPENTANONE	1757422		5.0		4.0*						1.0*								
180	2-HEXANEAMINE	5329793		5.0																

(Continued)

TABLE 10. (Continued)

COMBINED CONCENTRATE REPORT(PART I.A)

	COMMON NAME	CAS NO.	VLC	XLC	L2P	L2H	L2N	L2D	C3C	C1P	C1M	C1N	C2M	R1C	R2C	E1C	O2N	O2C	B1M	B1N
			RELATIVE SIZE																	
181	2,4-HEXADIEN-1-OL	111284		5.0																
182	5-PHENYL PENTANOIC ACID	2270204			4.0	5.0														
183	1,1-DIMETHYL TETRALIN	1985597			5.0															
184	4-ETHYL-1,2-DIMETHYL BENZENE	934805			5.0				1.0	3.0										
185	1,3-DISOPROPYL BENZENE	99627			5.0				1.0											
186	%*O-CHLOROANILINE	95512			3.2			2.0	2.0	3.0	5.0					1.0				
187	1,4-DIETHYL BENZENE	105055			5.0															
188	%P-CYMENE (P-ISOPROPYL TOLUENE)	99876			5.0							2.0								
189	ISODURENE	527537			5.0				1.0	3.0										
190	1-PHENYL DECANE	104723			5.0															
191	TRIMETHYLNAPHTHALENE	314			3.0		2.0		1.0	5.0										
192	DIBUTYL SEBACATE	109433			5.0															
193	2-(4-TERT-BUTYL PHENOXY)ETHANOL	713462			5.0															
194	1-METHYL-4-(1-METHYLETHYL)-3-CYCLOHEXEN-	586823			5.0															
195	N,N-DI-N-BUTYL FORMAMIDE	761659			5.0															
196	ISOPROPYL PHENYL PROPAN-1-OL	54518115			5.0										3.0					
197	%DIMETHYL PHTHALATE	131113			5.0				4.0			1.0		4.0	4.0	2.0		4.0	4.0	
198	4-TERPINEOL ISOMER	527			5.0					5.0										
199	TRIPROPYLENE GLYCOL, ETHYL ETHER ISOMER	20178341			5.0			1.0												
200	M-CYCLOHEXYLPHENOL	1943959			5.0											4.0		1.0		
201	%HYDROCINNAMIC ACID	501520				3.0	3.0						5.0				2.0			
202	2-METHYLBUTYRIC ACID	116530				3.0									4.0		1.0	3.0		5.0
203	2-ETHYLBUTYRIC ACID	88095				4.0		4.0				5.0							2.0	
204	%VALERIC ACID	109524				4.0	4.0	5.0			3.0		2.0	2.0	4.0			3.0	4.0	2.0
205	3-METHYL VALERIC ACID	105431				3.0		5.0			4.0								2.0	1.0
206	BIS(2-ETHOXYETHYL)ETHER	112367				5.0				3.0									3.7	
207	TETRAHYDROFURAN-2,5-DICARBOXYLIC ACID	2044880				5.0	4.0						3.0							
208	%*+PHENOL	108952				4.0	4.0	5.0	3.0	2.0	5.0	5.0	5.0					3.0	3.0	3.0
209	%*$P-CHLOROPHENOL	106489				1.0	1.0	3.0			5.0	6.0				2.0				
210	%ETHYL ACETATE	141786				5.0														
211	3,3 DIMETHYLGLUTARIC ACID	4839467				4.0	5.0													
212	%PENTABARBITAL	76744				3.0					5.0				4.0					
213	2,4,6-TRIMETHYLBENZOIC ACID	480637				2.0						5.0								
214	3-HEXANOL	623370				5.0			2.0					4.0	2.0			2.0	2.0	2.0
215	%METHYL ISOBUTYL KETONE	108101				5.0				5.0										
216	TRI-N-PROPYLENE GLYCOL, METHYL ETHER	13133294				5.0														
217	CYCLIC TETRAMETHYLENE ADIPATE	777957				3.0					5.0									
218	TETRAETHYLENE GLYCOL DIMETHYLETHER	143240				3.0	5.0	3.0							2.0					3.0
219	N-BUTYL ACETATE	123864				5.0														
220	2-(2-METHOXY-1-METHYLETHOXY)-1-PROPANOL	55956213				2.0	5.0												1.0	
221	BETA-CARYOPHYLLENE	13877935					5.0													
222	%ADIPIC ACID	124049					2.0						5.0							
223	TEREPHTHALIC ACID	100210					3.0	5.0										2.0		
224	METHYLCAPRYLIC ACID	504994					5.0													1.0
225	BETA-GURJUNENE	17334553					5.0													

(Continued)

TABLE 10. (Continued)

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COMBINED CONCENTRATE REPORT(PART I.A)

	COMMON NAME	CAS NO.	RELATIVE SIZE																	
			V1C	X1C	L2P	L2M	L2N	L2D	C3C	C1P	C1M	C1N	C2N	R1C	R2C	E1C	O2N	B2C	B1N	B1M
226	2,6-NAPHTHALIC ACID	1141384					5.0													
227	5-EPIDEOXYPODOCARPIC ACID	57345309					5.0			2.0	4.0									
228	CLOVENE	469921					5.0													
229	$M-CHLOROPHENOL	108430					4.0				5.0									
230	+ISOPHORONE	78591					5.0													
231	%N-NITROSO-3-METHYL PIPERIDINE	13603071					5.0													
232	NONYLPHENOL	25154523					5.0													
233	%MESITYL OXIDE (3-ISOHEXEN-2-ONE)	141797					5.0							4.0						
234	P-(2,2,3,3-TETRAMETHYLBUTYL)PHENOL	54932784					3.0			5.0										
235	2-ETHYLVALERIC ACID	2005						5.0						2.0					2.0	
236	2-METHYLGLUTARIC ACID	617629						5.0					4.0							
237	5-METHYL HEXANOIC ACID	628466						5.0	2.0					2.0			4.0		2.0	
238	2,6-DIMETHYLBENZOIC ACID	632462						5.0				4.0	5.0							
239	2,3,6-TRIMETHYL BENZOIC ACID	2529364						5.0												
240	%DICAMBA	1918009						5.0												
241	1-NAPHTHOIC ACID	86555						5.0											2.0	
242	3-(3,4-DIMETHOXYPHENYL)-2-PROPENOIC ACID	2316269						5.0												
243	2-METHYLCAPROIC ACID	4536236						5.0												
244	BETA,BETA-DIMETHYLPHENYLACETIC ACID	826551						5.0							4.0					
245	ALPHA-METHYLENE BENZENE PROPANOIC ACID	5076						5.0												
246	(2,5-DIMETHYLBENZENE)BUTANOIC ACID	1453061						4.0						4.0	4.0	1.0	3.0	5.0		
247	PHTHALIDE	87412						4.0			4.0	5.0			2.0				2.0	
248	2,2,4,4-TETRAMETHYL PENTANOIC ACID	3302123							4.0		4.0	3.0	5.0	3.0	3.0				3.0	
249	3-METHOXY-1,2-BENZISOTHIAZOLE	40991386							4.0		5.0									
250	*TRICRESYL PHOSPHATE (ISOMER UNKNOWN)	1330785							2.0						1.0			5.0		
251	DECYLENE	872059								5.0										
252	1-UNDECENE	821954								5.0										
253	ALPHA-DODECYLENE	112414								5.0										
254	%CYCLOHEXENE	110838								5.0										
255	2,3,6-TRIMETHYLNAPHTHALENE	829265								5.0	1.0	1.0			1.0					
256	1,3,6-TRIMETHYLNAPHTHALENE	3031081								5.0	2.0	1.0								
257	P-ISOPROPYLDIPHENYL AMINE	5650102								5.0										
258	9,10-DIHYDROPHENANTHRENE	776352								5.0										
259	2,2,5,7-TETRAMETHYL-4,5-OCTADIENE-3-ONE	19377970								5.0					2.0					
~~260~~	~~%CHLOROFORM~~	~~67663~~									~~5.0~~									
261	METHYL N-AMYL KETONE	110430									4.0				2.2			5.0		
262	2-METHOXY-4-METHYL-2-PENTENOIC ACID	1009									5.0	4.0							3.0	4.0
263	%N-UNDECYLIC ACID	112378									3.0			5.0	4.0			3.0		
264	TRANS-9-HEXADECENOIC ACID	373499									4.0	5.0								
265	1,2-BENZISOTHIAZOL-3(2H)-ONE	2634335									5.0								3.0	
266	1,3-DIMETHYL BUTABARBITAL	77281									5.0									
267	1-PHENYL-1,2,3-PROPANETRIOL	16354953									5.0									
268	%BENZYL ALCOHOL	100516									2.0			4.0	5.0		3.2	3.3	4.3	2.2
269	1-HEPTADECANOL	1454859									5.0						1.0			
270	%*2,4-DICHLOROPHENOXYACETIC ACID, (2,4-D)	94757										5.0			1.0		2.0			

(Continued)

TABLE 10. (Continued)

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COMBINED CONCENTRATE REPORT(PART I.A)

	COMMON NAME	CAS NO.	RELATIVE SIZE																	
			V1C	X1C	L2P	L2M	L2N	L2D	C3C	C1P	C1M	C1N	C2N	R1C	R2C	E1C	D2M	B2C	B1M	B1N
271	XBICHLORACETIC ACID	79436										5.0	5.0							
272	2-(2-METHOXYPROPOXY)-1-PROPANOL (A DIPR	13588288										3.0	5.0						3.0	
273	3-METHYL-2-HEPTANOL	31367461										5.0							3.0	
274	2-(2-HYDROXYPROPOXY)-1-PROPANOL (A DIPRO	106627										5.0			2.0					
275	~~1,2-CYCLOBUTANEDICARBOXYLIC~~ SEE NO. 50	~~1124136~~										~~5.0~~								
276	XMETHYL CHLOROFORM	71556										5.0								
277	2,2-DIMETHYL-1-BUTANOL	1185337										5.0								
278	~~SUBERANE~~	~~291645~~										~~5.0~~								
279	2-TERT-BUTYLCYCLOHEXANOL	13491797											5.0							
280	CHRYSANTHEMIC ACID	10453891											5.0							
281	2-ETHYL-3-METHYLFUMARIC ACID	28098808											5.0							
282	ETHENYL CYCLOPENTANEACETATE	45955666											5.0						3.0	
283	XARACHIDONIC ACID	506309												3.0	5.0					
284	ANTEISOPENTADECANOIC ACID	5502943												3.0	5.0		3.0			3.0
285	TRIPROPYLENE GLYCOL, METHYL ETHER	10213771												5.0					3.0	
286	XP-METHOXY-T-BUTYL PHENOL	25013165												5.0						
287	3-BUTYL-6-METHYL-2,4-PYRIDINEDIOL	6967700												5.0						
288	2-HYDROXY DECANOIC ACID	5393817													5.0		3.0	4.0		
289	1-((2,6,6-TRIMETHYL-1-CYCLOHEXEN-1-YL)OX	254													5.0					
290	TETRAETHYLENE GLYCOL MONOBUTYL ETHER	218													5.0					
291	8,11-OCTADECADIENOIC ACID	2197526													5.0				5.0	5.0
292	LIGNOCERIC ACID	557595													5.0					3.0
293	1,2 4,5-DI-O-ISOPROPYLIDENE-ALPHA-D-FRUC	28880937													5.0					
294	MYRISTYL ALCOHOL	112721															5.0			
295	3-METHOXY-2-BUTANOL	53778720																5.0		
296	CYCLOHEXYL FORMATE	4351546																1.0	5.0	
297	XMETA-CRESOL	108394																2.0	5.0	
298	1,5-BIS(T-BUTYL)-3,3-DIMETHYL BICYCLO(3.	1977956																5.0		
299	DIOCTYL AZELATE	103242																5.0		
300	OCTADECATRIENOIC ACID	4906916																	5.0	5.0
301	ACENAPHTHYLENE	208968																	5.0	2.0
302	PIPERIDINOL	6459990																	5.0	
303	XMETHYLPHENYL CARBINOL	98851																	5.0	
304	1-CYCLOPENTYLETHANONE	6004600																		5.0
305	7-OCTEN-2-ONE	3664606																		5.0
306	XS1,2-DICHLOROETHANE	107062			4.6								4.0							
307	4-HYDROXY-4-METHYLCYCLOHEXANONE	17429026																	4.6	4.6
308	X*P-CRESOL	106445	0.2															4.2*	4.0*	3.0*
309	XCYCLOHEXANOL	108930		4.2		2.0*									4.0*		2.1*		4.0*	3.0*
310	1,2 5,6-BIS-O-ISOPROPYLIDENE-BETA-D-TALO	23262795		4.2																
311	BUTYL CLOFIBRATE	1713140						4.2												
312	2-BUTYL THF	1004291										4.2						2.0		
313	XCAFFEINE	58082				4.0	4.0	4.1				3.0		3.0						
314	XDMF (DIMETHYLFORMAMIDE)	68122					2.0				4.1	2.0	3.2				2.0			
315	PHTHALIC ANHYDRIDE	85449						3.0							4.1		1.0			

(Continued)

TABLE 10. (Continued)

COMBINED CONCENTRATE REPORT(PART I.A)

	COMMON NAME	CAS NO.	RELATIVE SIZE V1C	X1C	L2P	L2M	L2N	L2D	C3C	C1P	C1M	C1N	C2N	R1C	R2C	E1C	O2N	B2C	B1M	B1N
316	N-ACETYLCYCLOHEXYLAMINE	1124534																		
317	4,4-DIMETHYLDIHYDROFURANONE	13861977													4.1					
318	2-METHOXY-1-PROPANOL	1589475	0.0																4.1	1.0
319	ISOMYRISTIC ACID	543	0.0											4.0*				2.0*		
320	9-KETOCAPRIC ACID	1422260	-1.0												4.0*					
321	ISOPALMITIC ACID	545	-1.0											3.0*	4.0	2.0*	4.0	3.0*		
322	%*+$FLUORANTHENE	206440	-2.0		1.0*					4.0	1.0*				4.0					
323	3,4-EPOXY-2-HEXANONE	17257817	2.0												2.0*				1.0*	
324	%$TOLUENE	108883		3.0	4.0*	1.0*						4.0*				3.0*				
325	DIACETONE ALCOHOL	123422		3.0		2.0*							4.0*			4.0*				
326	%CETYL ALCOHOL	36653824		2.0								3.0*		4.0*					2.0*	
327	METHYL AMYL CARBINOL	543497		4.0													4.0*			
328	4-HEPTANONE	123193		4.0		3.0*			3.0*				2.0*					4.0*	3.0*	
329	(1,4-CYCLOHEXADIEN-1-YL)BENZENE	13703521		4.0								2.0*								
330	4-METHYL DIOXANE	1120974			4.0															
331	2-ACETYL-4-METHYL-4-PENTENOIC ACID	1005			3.0															
332	%$BUTYL(BUTOXY CARBONYL) METHYL PHTHALATE	85701			4.0	4.0							4.0							
333	O-ETHYL TOLUENE	611143			4.0				2.0	3.0	2.0	2.0								
334	%*$STYRENE	100425			4.0	2.0	1.0	0.0	1.0	2.0	1.0	2.0			1.0		1.0			
335	(1,1-DIMETHYLBUTYL) BENZENE	1985575			4.0															
336	6-METHYL TETRALIN	1680519			4.0					1.0										
337	PSEUDOCUMENE	95636			3.0			0.0	3.0	4.0	2.0	2.0	1.0		1.0					
338	2-ETHYL-1,3-DIMETHYL BENZENE	2870044			4.0															
339	1-METHYL INDAN	767588			4.0															
340	%2-METHYLNAPHTHALENE	91576			2.0			0.0	2.0	4.0	2.0	1.0		1.0	1.0				4.0	
341	1-ETHYL-3,5-DIMETHYL BENZENE	934747			4.0				1.0	3.0										
342	2-BUTYLNAPHTHALENE	1134629			1.0		1.0			4.0	1.0									
343	P-DIISOPROPYL BENZENE	100185			4.0															
344	C5 BENZENE	120			4.0															
345	2-METHYL TETRALIN	3877198			4.0															
346	%BIPHENYL	92524			2.2	1.0	1.0	0.0		3.1	4.0	2.0	2.0	1.0	3.1		2.0		1.0	
347	DIMETHYL NAPHTHALENE	300			3.0		1.0		1.0	4.0	2.0									
348	%O-CRESOL	95487			2.0			2.0		2.0										
349	1-METHYLPYRENE	2381217			4.0														4.0	
350	TERPHENYL	26140603			4.0															
351	2,3,5-TRIMETHYL PHENANTHRENE	3674735			4.0															
352	1-METHYL ANTHRACENE	610480			2.0					4.0										
353	2-OCTYLPHENOL	949133			4.0				2.0	4.0										
354	EXO-BORNEOL	124765			2.0															
355	%ENDO-BORNEOL	507700			4.0														4.0	
356	%CAMPHOR	76222			4.0										3.0					
357	FENCHYL ALCOHOL	1632731			4.0															
358	DI-T-BUTYL ETHER	6163662			4.0															
359	CIS-1,2-CIS-2,3-PLINOL	11039728			4.0															
360	2-(2-ISOPROPYLPHENYL)-1-PROPANOL	58443826			4.0															

(Continued)

TABLE 10. (Continued)

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COMBINED CONCENTRATE REPORT(PART I.A)

	COMMON NAME	CAS NO.	RELATIVE SIZE																	
			V1C	X1C	L2P	L2M	L2N	L2D	C3C	C1P	G1N	C1N	G2N	R1C	R2C	E1C	D2N	B2C	B1M	B1N
361	CIS-2-METHYLCYCLOPENTANOL	25144052			2.0	4.0						2.0					1.0		1.0	
362	TRIOCTYL PHOSPHATE	1806548			4.0					4.0										
363	METHYL HENEICOSANOATE	6064900			4.0															
364	METHYLDEHYDROABIETATE	1235741			4.0										3.0					
365	BENZOFURANONE	7169348			2.0		1.0				4.0									
366	METHYL OCTENOATE	700			4.0															
367	3-OCTENOIC ACID	1577191				4.0														
368	$DIMETHYL TEREPHTHALATE	120616				4.0			2.0											
369	2-CYCLOHEXENONE	930687				2.0						4.0	2.0	3.0						2.0
370	2,5-HEXANEDIONE	110134				3.0		2.6			3.0	4.0	2.0	2.0		4.0	0.0		1.0	0.0
371	DIETHYLENE GLYCOL, MONOMETHYL ETHER (C	111900				3.0		1.0	1.0		4.0				1.0					3.0
372	3,5,5-TRIMETHYLCYCLOHEX-3-EN-1-ONE	471012				2.0	4.0	3.0												
373	DICYCLOHEXYLADIPATE	849990				1.0														4.0
374	P-(1,1,3,3-TETRAMETHYLBUTYL)PHENOL	140669				1.0	4.0	1.0		3.0	4.0	4.0								
375	CHLOROBENZOIC ACID ISOMER	708					4.0													
376	ALPHA-CARYOPHYLLENE	6753986					4.0													
377	ISO-HEXANOIC ACID	646071					3.0					4.0		2.0						
378	4,5-DIMETHYL-1-HEXENE	16106595					4.0													
379	2,3-DIMETHYLBUTYRIC ACID	14287617					3.0	4.0											2.0	1.0
380	%+ANTHRACENE	120127					1.0	0.0	1.0	4.0										
381	~~DOCOSANE~~	~~629970~~					4.0													
382	1-SEC-BUTOXY-2-METHOXYPROPANE	1001					4.0													
383	3-METHYL-2-CYCLOHEXEN-1-ONE	1193186					3.0	3.0											4.0	2.0
384	4,4,5-TRIMETHYL-2-CYCLOHEXEN-1-ONE	17429297					4.0													
385	VINYL CYCLOHEXYLFORMATE	4840760					3.0	4.0					2.0							3.0
386	P-(1-ETHYL-1-METHYLHEXYL)PHENOL (A NONY	52427131					4.0													
387	DIMETHYLSULFONE	67710					3.0	3.6			4.0	2.0	2.0	3.0	2.0		1.0		2.0	2.6
388	2-(2-METHOXY-1-METHYLETHOXY)-2-PROPANOL	55956224					1.0													4.0
389	%BUTYRIC ACID	107926						4.0												
390	4,4-DIMETHYL-2-PENTENOIC ACID	6945353						4.0				3.0								
391	4-OCTENOIC ACID	18294898						4.0							3.0					
392	N-BENZOYLGLYCINE (HIPPURIC ACID)	495692						4.0												
393	4,6,6-TRIMETHYLTETRAHYDRO-2-PYRANONE	20628368						4.0					3.0							
394	5-BUTYLDIHYDRO-2-FURANONE	34003775						4.0												
395	TRIETHYLENE GLYCOL, DIMETHYL ETHER	112492						4.0				3.0							2.0	
396	$TERT-BUTYL METHYL PHTHALATE	1007							4.0											
397	DIMETHYLNAPHTHALENE	301							2.0	4.0										
398	1,5,8-TRIMETHYL TETRALIN	21693516							1.0	4.0										
399	%2-HYDROXYBIPHENYL	90437							4.0											
400	3-OCTANONE	106683							4.0											
401	1-OCTENE	111660								4.0										
402	1-NONYLENE	124118								4.0										
403	SEBACIC ACID	111206								4.0							3.0			
404	1-TRIDECENE	2437561								4.0							0.0			
405	1-TETRADECENE	1120361								4.0										

(Continued)

TABLE 10. (Continued)

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COMBINED CONCENTRATE REPORT(PART I.A)

	COMMON NAME	CAS NO.	RELATIVE SIZE																	
			V1C	X1C	L2P	L2M	L2N	L2D	C3C	C1P	C1M	C1N	C2N	R1C	R2C	E1C	D2N	B2C	B1M	B1N
406	1-PENTADECENE	13360617								4.0										
407	CETENE	629732								4.0							2.0			
408	2-METHYL-2-PROPYLHEXANOIC ACID	31080372								3.0	4.0									
409	2,6-DIISOPROPYLPHENOL	2078548								4.0										
410	%3,4-DICHLOROANILINE	95761								4.0										
411	1,3,8-TRIMETHYLNAPHTHALENE	17057919								4.0										
412	1,2,3-TRIMETHYL-4-PROPENYLNAPHTHALENE (T	26137531								4.0										
413	1,4,6-TRIMETHYL NAPHTHALENE	2131422								4.0				2.0	1.0					
414	BUTYLATED HYDROXY ANISOLE (BHA)	15359996								4.0					3.0					
415	1,4,6-TRIMETHYL TETRALIN	22824324								4.0										
416	N-PROPYLSUCCINAMIDE	3470971								4.0										
417	METHYL PALMITOLEATE	1120258								4.0										
418	%ISOBUTYRIC ACID	79312									4.0		4.0							
419	2-METHOXY-3-METHYL-2-PENTENOIC ACID	1008									4.0	3.0							4.0	3.0
420	CIS-2,5-DIMETHYLTETRAHYDROFURAN	2144414									4.0									
421	N-METHYLETHOSUXIMIDE	13861999									4.0									
422	%*+$2,4-DICHLOROPHENOL	120832									4.0				1.0			1.0		
423	4-TERT-BUTYL-O-PHENYLENE CYCLIC CARBONAT	54815213									4.0									
424	BUTABARBITAL	125406									4.0									
425	ANISOLE-2-ACETIC ACID	93254									4.0									
426	BETA,3,4-TRIMETHYLBENZENEPROPANOIC ACID	1011									4.0									
427	2-(PHENYLMETHYL)BENZOIC ACID	612351									4.0									
428	2,2-DIMETHYLGLUTARIC ACID	681572									4.0		4.0							
429	%P-TERT-BUTYL PHENOL	98544									4.0									
430	1,3-DIMETHOXY-2-PROPANOL	623698									4.0									
431	1,3-PROPYLENE GLYCOL, BUTYL METHYL DIETH	1012									4.0									
432	%CHLOROBENZENE	108907										4.0			0.0					
433	3-METHOXY-2-METHYL-2-PENTENOIC ACID	1014										4.0								
434	ALPHA,ALPHA-DICHLOROPHENYLACETIC ACID	61031729										4.0				2.0				
435	1-(2-BUTOXY-1-METHYLETHOXY)-2-PROPANOL (	29911282										4.0								
436	6-METHYL-TETRAHYDRO-2-PYRANONE	823223										4.0								
437	HEXAHYDRO-4-METHYL-2H-AZEPIN-2-ONE	3623050										4.0								
438	6-METHYL-3(2H)-BENZOFURANONE	20895414										4.0	3.0							
439	~~3,3-DIETHYLPENTANE~~	~~1067205~~										~~4.0~~								
440	1-METHOXY-2-HEXENE	56052836										4.0								
441	DI-N-HEXYL ETHER	112583										4.0								
442	ACETOACETIC ACID	541504											4.0							
443	1-METHOXY-2-BUTANOL	53778737											4.0							
444	2,3-DIMETHYL-3-PENTANOL	595415											4.0							
445	2,6-DIMETHYLPHENOXY CARBONIC ACID	1013											4.0							
446	2-METHYLCYCLOPENTANOL (GEOMETRY UNKNOWN)	24070777											4.0					3.0		
447	%6-HYDROXYCAPROIC ACID LACTONE	502443											4.0							
448	2-(HYDROXYMETHYL)BENZOIC ACID	612204											4.0				2.0			
449	TRIDECYLIC ACID	638539												3.0	4.0		2.0			
450	UNDECANEDIOIC ACID	1852046												4.0	4.0		4.0	3.0		

(Continued)

TABLE 10. (Continued)

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COMBINED CONCENTRATE REPORT(PART I.A)

	COMMON NAME	CAS NO.	RELATIVE SIZE																	
			V1C	K1C	L2P	L2M	L2N	L2D	C3C	C1P	C1M	C1N	C2N	R1C	R2C	E1C	D2N	B2C	B1M	B1N
451	4-BUTOXYBUTYRIC ACID	55724737												3.0					4.0	
452	3-HEPTANOL	589822												3.0				4.0	2.0	
453	2,3-DIMETHYLTETRAHYDRO-2-FURANOL	61142776												3.0				4.0		
454	6-BROMO-2-HEXANONE	10226296												3.0		3.0		4.0		
455	%TRIMETHYL NITROSO UREA	3475636												4.0						
456	3,4-DIHYDROXY-6-METHOXY-1-NAPHTHALENONE	1078199												4.0						
457	BUTYLBENZYLPHTHALATE	38411120												4.0						
458	%BENZYL CYANIDE	140294												4.0	3.0			1.0		
459	PIPERIDINONE	27154434												4.0						2.0
460	1-ETHOXY DECALIN	51953107													4.0					
461	4-OXO-NONANOIC ACID	6064524													4.0		3.0			
462	VACCENIC ACID	693721													4.0					
463	NONADECANOIC ACID	646300													4.0					
464	BEHENIC ACID	25378261													4.0					2.0
465	1,3,6-TRIOXOCANE	1779197													4.0					
466	2-ETHYL-1,3-HEXANEDIOL	94962													4.0					
467	2-ETHYL-5-METHYLDIOXANE	53907918													4.0					
468	% PYRIDINE	110861													4.0					
469	ETHYL PALMITATE	628977													4.0					
470	4-HEXEN-2-ONE	25659227														4.0				
471	5-METHYL-2-HEXANOL	627598														4.0				
472	3-HYDROXY-1,2-BENZISOTHIAZOLE	3434																4.0		
473	2,6-DICHLOROBENZOIC ACID	50793																4.0		
474	O-PROPIONYL BENZOIC ACID	4219550																4.0		
475	2-METHYL-4-DIBROMOMETHYL BENZOIC ACID	129																4.0		
476	3-HYDROXYTETRADECANOIC ACID	1961724																4.0		
477	%ANTHRANILIC ACID	118923																	4.0	
478	2-AMINO-5-CHLOROBENZOIC ACID	89543																	4.0	
479	4-HYDROXY-4-METHYL-2-PENTANONE	123442																	4.0	2.0
480	2,2,3-TRIMETHYL-3-CYCLOPENTENE-1-ACETALD	4501580																	4.0	
481	2,3-BUTANEDIOL	513839																		4.0
482	O-ANISIC ACID	579759																		4.0
483	3-METHOXYBENZOIC ACID	586389																		4.0
484	TERPIN	80535																	3.2	4.0
485	DICYCLOHEXYL SEBACATE	366																		4.0
486	%CINNAMALDEHYDE	104552										3.6								
487	%N-METHYL-2-PYROLIDONE	872504				1.0													2.0	3.2
488	~~%TERPIN~~ SEE NO. 484	~~2451016~~																	~~3.2~~	
489	BUTYLBENZOATE	136607			3.0									3.1	3.0			2.0		
490	DIDEHYDROGENATED ABIETIC ACID	625	0.0														1.0*	3.0*	3.0*	
491	3-METHYLPENTAN-3-OL	77747	0.0			3.0*						2.0*								
492	P-(1-HYDROXY-1-METHYLETHYL)ACETOPHENONE	54549723	0.0											3.0*						
493	METHYL MYRISTATE	124107	1.0		3.0*					3.0*					2.0*					
494	1,2-BENZISOTHIAZOLE	272162	1.3												3.0*					
495	N-PROPYL-1-HEXANAMINE	20193231	-1.0									3.0*								

(Continued)

TABLE 10. (Continued)

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COMBINED CONCENTRATE REPORT(PART I.A)

	COMMON NAME	CAS NO.	RELATIVE SIZE V1C	X1C	L2P	L2M	L2N	L2D	C3C	C1P	C1M	C1N	C2N	R1C	R2C	E1C	D2N	B2C	B1M	B1N
496	~~PHOSPHORIC ACID~~	~~456~~		~~3.0*~~																
497	3-PENTEN-2-OL	1569502		3.0													1.0*			2.0*
498	2-METHYLCYCLOPENTANONE	1120725		3.0		2.0*						2.0*							2.0*	1.0*
499	(1-METHYLBUTYL)OXIRANE	53229393		3.0																
500	OCTADECANOL	26762447		2.0											3.0*		2.0*			
501	8-NONENE-2-ONE	5009325		2.0												3.0*			3.0*	
502	%CHLOROBROMOMETHANE	74975			3.0	3.0														
503	2,4,6-TRIMETHYLUNDECANOIC ACID	28484222			3.0															
504	10-UNDECENOIC ACID	112389			3.0												1.0			
505	3-METHYLCYCLOHEXENE	591480			3.0															
506	%3-CHLORO-2-METHYL PROPENE	563473			3.0															
507	1,2-DICHLOROPENTANE	1674335			3.0															
508	1-CHLOROHEPTANE	629061			3.0															
509	ACETALDEHYDE DIETHYL ACETAL	105577			3.0													3.0		
510	3-PHENYL-3-METHYLHEXANE	2132867			3.0															
511	%$M-XYLENE	108383			3.0			0.0				3.0	3.0				1.0			
512	4-PHENYLCYCLOHEXENE	4994165			3.0															
513	1,2,3-TRIMETHYL BENZENE	526738			3.0			0.0	2.0	3.0	2.0	1.0			0.0					
514	%MESITYLENE	108678			3.0			0.0	2.0	3.0		2.0								0.0
515	1-METHYL-2-PROPYL BENZENE	1074175			3.0															
516	4-METHYL INDAN	824226			3.0															
517	%1-METHYLNAPHTHALENE	90120			3.0			0.0	1.0	3.0	2.0	1.0		1.0	1.0				0.0	
518	%2-ETHYL NAPHTHALENE	939275			2.0		1.0		1.0	3.0										
519	%1,4-DIMETHYLNAPHTHALENE	571584			3.0					3.0										
520	1,6,7-TRIMETHYLNAPHTHALENE	2245387			2.0					3.0	1.0	1.0								
521	1-ETHYL-2,4-DIMETHYL BENZENE	874419			3.0					3.0										
522	1-ETHYL-2,3-DIMETHYL BENZENE	933982			3.0					2.0										
523	%$CUMENE	98828			3.0				1.0	1.0										
524	1-METHYL-4-PROPYLBENZENE	1874551			3.0							1.0								
525	N-BUTYLBENZENE	104518			3.0					2.0			1.0							
526	2-PHENYLPENTANE	2719520			3.0															
527	C5 BENZENE	121			3.0															
528	%+$O-DICHLORO BENZENE	95501			2.0				1.0	3.0							0.0			
529	DIMETHYL INDAN	615			3.0															
530	DIMETHYL ISOPROPYL BENZENE	103			3.0															
531	ETHYL TRIMETHYL BENZENE	114			3.0															
532	4,7-DIMETHYL INDAN	6682719			3.0					1.0										
533	DIMETHYL INDAN	616			3.0															
534	2,7-DIMETHYL TETRALIN	13065071			3.0															
535	1-PHENYL NONANE	1081772			3.0															
536	%2,6-DIMETHYLNAPHTHALENE	581420			3.0				2.0		2.0									
537	1,6-DIMETHYLNAPHTHALENE	575439			3.0			0.0			1.0			1.0	2.0					
538	1-PHENYL UNDECANE	6742547			3.0															
539	DIISOPROPYL PHENOL	520			3.0										3.0					
540	TRIMETHYLNAPHTHALENE	311			3.0		2.0		1.0			1.0			1.0					

(Continued)

TABLE 10. (Continued)

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COMBINED CONCENTRATE REPORT(PART I.A)

	COMMON NAME	CAS NO.	RELATIVE SIZE																	
			V1C	X1C	L2P	L2M	L2N	L2D	C3C	C1P	C1M	G1N	G2N	R1C	R2C	E1C	O2N	B2C	B1M	B1N
541	TRIMETHYLNAPHTHALENE	312			3.0		2.0		1.0											
542	TRIMETHYLNAPHTHALENE	313			3.0		2.0		1.0								0.0			
543	DIMETHYL BIPHENYL	600			3.0															
544	(1,1-DIMETHYLPROPYL)BENZENE	2049958			3.0					2.0										
545	1-ETHYL-3-METHYL BENZENE	620144			1.0				2.0	3.0	1.0									
546	2-ISOPROPYLNAPHTHALENE	2027170			3.0					3.0										
547	XRETENE	483658			3.0		3.0													
548	2-(PHENYLMETHYL) NAPHTHALENE	613592			3.0															
549	DURENE	95932			1.0				1.0	3.0	1.0	1.0								
550	DIMETHYL ETHYL BENZENE	208			2.0					3.0										
551	DIMETHYL ETHYL BENZENE	201			1.0					3.0										
552	XCINEOLE	478826			3.0														3.0	
553	XMETHYL BENZOATE	93583			2.0		3.0													
554	B-PICOLINE	108996			3.0															
555	N,N-DIETHYL FORMAMIDE	617845			1.0									3.0						
556	FENCHONE	1195795			3.0	3.0														
557	2-ETHOXYETHYL-2-BUTOXYETHYL ETHER	3095178			3.0															
558	XTRICHLOROPROPANE	96184			3.0															
559	XACETOPHENONE	98862			2.0	2.0		3.0		1.0	2.0	3.0	2.6				0.0			
560	DIHYDRO FARNESOL	1335484			3.0															
561	XNICOTINE	54115			3.0		2.0				3.0				2.0					
562	~~3,4-DIMETHYL HEXANE~~	~~589435~~				~~3.0~~														
563	2-METHYL VALERIC ACID	97610				2.0		3.0					3.0							
564	ISOPROPYL BENZOATE	939480				3.0														
565	3-METHYL-4-PHENYLBUTYRIC ACID	7315686				3.0														
566	1,6 DIMETHYL-4-ISOPROPYL-NAPHTHALENE	483783				2.0	3.0	0.0	1.0			2.0			2.0		1.0			
567	XTRIETHYL PHOSPHATE	78400				2.0													3.0	
568	XCYCLOHEXANONE	108941				1.0											1.0		3.0	2.0
569	VINYL ACETATE	108054				3.0														
570	MENTHONE	10458147				3.0														
571	COTININE	486566				1.0									3.0					
572	ANISIC ACID	100094					3.0									1.0	2.0	2.0		
573	XGLUTARIC ACID	110941					3.0													
574	AMINOPHTHALAZINE	19064698					3.0													
575	3-METHYLGLUTARIC ACID	626517					3.0													
576	XDALAPON	75990					3.0													3.0
577	~~EICOSANE~~	~~112958~~					~~3.0~~													
578	~~7-HEXYLTRIDECANE~~	~~7225663~~					~~3.0~~													
579	1,1,3-TRIMETHYL-3-PHENYL INDAN	3910358					3.0					1.0								
580	TRICOSANE	638675					3.0													
581	~~TETRACOSANE~~	~~646311~~					~~3.0~~													
582	~~PENTACOSANE~~	~~629992~~					~~3.0~~													
583	TETRAHYDROLINALOOL	78693					3.0		1.0											
584	METHYL HEPTADECANOATE (METHYL MARGARAT	1731926					3.0													
585	5,5-DIMETHYL-2-FURANONE	20019641					2.0	3.0											3.0	2.0

(Continued)

TABLE 10. (Continued)

COMBINED CONCENTRATE REPORT(PART I.A)

	COMMON NAME	CAS NO.	RELATIVE SIZE																	
			V1C	X1C	L2P	L2M	L2N	L2D	C3C	C1P	G1M	C1N	C2N	R1G	R2C	E1G	O2N	O2C	O1M	O1N
586	3,5-DIMETHYL-2-CYCLOHEXEN-1-ONE	1123097					3.0	3.0												
587	1-INDANONE	83330					3.0					3.0								
588	ISONONYL PHENOL (ISOMER UNKNOWN)	11066492					3.0													
589	P-(1-METHYLOCTYL)PHENOL (A NONYL PHENOL	17404669					3.0													
590	TRIETHYLENE GLYCOL METHYL ETHER	112356					3.0													
591	%+*2,4-DIMETHYLPHENOL (XYLENOL)	105679						1.0											3.0	1.0
592	2-HEXENOIC ACID	1191044						3.0												
593	DIETHYL KETONE	96220						3.0												
594	METHYL ISOPENTYL KETONE	110123						3.0												
595	1-(1-CYCLOHEXEN-1-LY)-2-PROPANONE	768503						3.0												
596	2-BUTYL-3-METHYLOXIRANE	14925963						3.0				3.0								
597	3,5,5-TRIMETHYL-2-CYCLOPENTEN-1-ONE	24156954						3.0												
598	5-ETHYLDIHYDRO-2(3H)-FURANONE	695067						3.0			3.0						1.0		2.0	2.0
599	6-METHYL-3-ISOPROPYL-2-CYCLOHEXEN-1-ONE	499741						3.0												
600	5-PHENYL-2-PENTANONE	2239838						3.0												
601	OCTYL PHENOL	500						3.0												
602	5-(PENTYLOXY)-2-PENTENE	56052058						3.0												
603	.ALPHA.-HYDROXY-.ALPHA.-METHYL BENZENE A	515300						3.0												
604	1-PHENYL-2-BUTANONE	1007325						3.0												
605	2-BUTYLOCTANOL	3913028						3.0												
606	5-METHYL-1(3H)-ISOBENZOFURANONE	54120648						3.0												
607	ISOVALERAMIDE	541468						1.0						3.0						
608	HEXAHYDRO-2H-AZEPINE-2-ONE	105602						1.0												3.0
609	P-CHORO-2-NITROANILINE	89634						3.0												
610	ETHYLPHENOXYBENZENE	834140						3.0												
611	%MALONIC ACID	141822							3.0											
612	4-METHYLPHENYLPENTANOIC ACID	59094712							3.0											
613	$ISOBUTYL METHYL PHTHALATE	1004							3.0											
614	$SEC-BUTYL METHYL PHTHALATE	1006							3.0											
615	2-ETHYL-1,4-DIMETHYL BENZENE	1758889							1.0	3.0										
616	%+$M-DICHLOROBENZENE	541731							1.0			3.0								
617	METHYL METHOXYMETHYL FORMAL	628980							3.0											
618	%2,6-LUTIDINE	108485							2.0		3.0			2.0	1.0					
619	%M-CHLOROANILINE	108429							3.0	3.0										
620	%$2,3,4,6-TETRACHLOROPHENOL	58902								3.0										
621	%$2,4,5-TRICHLOROPHENOL	95954								3.0										
622	META-TERT-BUTYLPHENOL	585342								3.0										
623	ETHYLENE GLYCOL, MONOMETHYL ETHER	109864								3.0							2.0	3.0		
624	~~BICYCLO(2.2.2) OCTANE~~	~~280331~~								~~3.0~~										
625	1,5-DIMETHOXYPENTANE	111897								3.0										
626	~~BICYCLO DECANE~~	~~286760~~								~~3.0~~										
627	1-HEPTADECENE	6765395								3.0										
628	1-OCTADECENE	112889								3.0							2.0			
629	1,3-BUTYLENE GLYCOL	107880								3.0										
630	PENTAMETHYLENE GLYCOL, MONOMETHYL ETHER	4799626								3.0										

(Continued)

TABLE 10. (Continued)

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COMBINED CONCENTRATE REPORT(PART I.A)

	COMMON NAME	CAS NO.	V1C	X1C	L2P	L2M	L2N	L2D	C3C	C1P	C1M	C1N	C2N	R1C	R2C	E1C	D2M	D2C	B1M	B1N
			RELATIVE SIZE																	
631	METHYL-N-PROPYLBENZENE	205								3.0										
632	METHYL-N-PROPYLBENZENE	206								3.0										
633	2,7-DIMETHYLNAPHTHALENE	582161								3.0										
634	1,2,8-TRIMETHYLNAPHTHALENE (3,4,5-TR	3876979								3.0		1.0								
635	DIMETHYLNAPHTHALENE	302								3.0										
636	1,3-DIMETHYNAPHTHALENE	575417								3.0		2.0			1.0					
637	OCTENAL (ISOMER UNKNOWN)	25447692								3.0										
638	O-CYCLOHEXYLPHENOL	119426								3.0										
639	%BORNYL ACETATE	76493								3.0										
640	%2,6-DIMETHYLQUINOLINE	877430								3.0					2.0					
641	SEC-BUTYLISOPROPYL ETHER	18641811									3.0									
642	2,6-DIMETHYLHEPTANOIC ACID	60148949									3.0		3.0		2.0		1.0			
643	2-METHOXY-3-METHYLCROTONIC ACID	58973185									3.0	2.0								2.0
644	3,6-DIMETHYLOCTANOIC ACID (AN ISODECANOI	4812297									3.0						2.0			
645	LEVULINIC ACID	123762									3.0	3.0								2.0
646	%2,2,2-TRICHLOROETHANOL	115208									3.0								2.0	
647	9-DODECENOIC ACID	2382403									3.0									
648	2,3,3-TRIMETHYL-3H-INDOLE	1640397									3.0									
649	$0-CHLOROPHENOL	95578									3.0									
650	%TETRAMETHYLUREA, THU	632224									3.0	2.0								
651	2,2,5,5-TETRAMETHYL THF	15045439										3.0								
652	4-KETOISOHEPTANOIC ACID	41654040										3.0								2.0
653	ALPHA-METHYL-ALPHA-ACETYLOXYBENZENEACETI	10487920										3.0								
654	2,5,8-TRIMETHYL-1-NAPHTHOL	33583027										3.0								
655	2,5-DIMETHYL STYRENE	2039896										3.0								
656	1-(3-BUTOXYPROPOXY)-2-PROPANOL (A DIPROP	35075242										3.0								
657	ALPHA-PICOLINE	109068										3.0								
658	%2-ACETYLFURAN	1192627										3.0	3.0							
659	3-METHYL PHTHALIDE	3453643										3.0								
660	7-METHYL-3(2H)-BENZOFURANONE	669845										3.0	3.0							
661	BUTYL M-TOLYL SULFIDE	54576419										3.0								
662	TETRAHYDROPYRAN-2-METHANOL	100721										3.0								
663	~~3-ETHYL-4-METHYLHEXANE~~	~~3074779~~										~~3.0~~								
664	~~2,7-DIMETHYLOCTANE~~	~~1072168~~										~~3.0~~								
665	2,2-DICHLORO-3-METHYLBUTANE	17773669										3.0								
666	1,6-HEXANEDIOL	629118										3.0								
667	2-NORBORNENE-7-OL	53783872										3.0								
668	2-HEXENAL	505577										3.0								
669	2,6-DIMETHYL-2-HEPTEN-4-ONE	16525056										3.0								
670	2,2-DIMETHYL-3-PENTANOL	3970625											3.0							3.0
671	4-METHYL-3-CYCLOHEXENE-1-CARBOXYLIC ACID	4342603											3.0							
672	2-ETHYL-2-METHYLBUTYRIC ACID	19889373											3.0							
673	4-METHYL-2-PHENYLQUINOLINE	4789768											3.0							
674	1-(PHENYLMETHYL)ISOQUINOLINE	6907591											3.0							
675	1,2,4-TRIMETHYL-1,3-DIAZOCYCLOHEX-1-ENE	53517923											3.0							

(Continued)

TABLE 10. (Continued)

COMBINED CONCENTRATE REPORT(PART I.A)

	COMMON NAME	CAS NO.	RELATIVE SIZE																	
			V1C	X1C	L2P	L2M	L2N	L2D	G3C	C1P	C1N	C1M	C2N	R1C	R2C	E1C	D2N	B2C	B1M	B1N
676	1-ACETYL-1,2,3,4-TETRAHYDROPYRIDINE	19615271											3.0							
677	DIETHYLENEGLYCOL, CYCLOHEXYL ETHER	25961046											3.0							
678	%DI-N-PROPYL PHTHALATE	131168											3.0							
679	7-NONENOIC ACID	1022												3.0			2.0			
680	ISOINDOLE-1,3-DIONE	85416												3.0						
681	2-ETHYL-3-METHYL-2-BUTENEDIOIC ACID	2007												3.0						
682	TRICOSANOIC ACID	2009												2.0	3.0					
683	NONACHLOR	21641703												3.0	2.0					
684	1-METHYLBUTYLALCOHOL	6032297												3.0						
685	%N-OCTANOL	111875												3.0	2.0					
686	%2-PHENYLISOPROPANOL	617947												3.0	3.0					
687	%1,2-DIHYDRO-3,6-PYRIDAZINEDIONE	123331												3.0						
688	5,6,7,7A-TETRAHYDRO-4,4,7A-TRIMETHYL-2(4	17092921												3.0						
689	3-ETHOXY-1(3H)-ISOBENZOFURANONE	16824025												3.0						
690	2-ISOPROPYLTHIOPHENE	1689787												3.0						
691	3-(2-HYDROXYPROPYL)-5-METHYL-2-OXAZALIDI	3375846												3.0	3.0					
692	3-METHYLOCTAHYDROPENTALENE-1-CARBOXYLIC	28645036													3.0					
693	4-HYDROXY-OCTAHYDRO-1-NAPHTHALENONE	33993349													3.0					
694	2,2-DIMETHYL-3-(2-METHYL-1-PROPENYL)CYCL	32511061													3.0					
695	4-ISOPROPOXYBUTYRIC ACID	146													3.0					
696	ISOSTEARIC ACID	5638120													3.0					
697	ISOEICOSANOIC ACID	3121													3.0					
698	VERATRALDEHYDE	120149													3.0					
699	HENEICOSANIC ACID	2363715													3.0					
700	PENTACOSANOIC ACID	506387													3.0					
701	HEXACOSANOIC ACID	506467													3.0					
702	1,2,4,5,6,7,8,8-OCTACHLORO-2,3,3A,4,7,7A	5103742													3.0					
703	NEOPENTYL ALCOHOL	75843													3.0					
704	4-METHOXY-5-METHYL-4-CYCLOPENTEN-1,3-DIO	7180623													3.0					
705	N-(2-METHYLPHENYL)FORMAMIDE	94699													3.0					
706	3-METHYLPENTANAL	15877573													3.0					
707	%LAURYL ALCOHOL	112538													2.0		3.0			
708	PENTYL BENZOATE	2049969													3.0					
709	TETRAPROPYLENE GLYCOL	1377													3.0					
710	TETRAPROPYLENE GLYCOL	1378													3.0					
711	TETRAPROPYLENE GLYCOL	1379													3.0					
712	%CHLOROACETONE	78955													3.0					
713	1,4-BENZOTHIAZIN-3-ONE	5325202														3.0	2.0			
714	5-METHYL-1-HEXANOL	627985														3.0				
715	HEXAHYDROBENZOIC ACID	98895															2.0			3.0
716	DODECANEDIOIC ACID	693232															3.0			
717	%ETHYLENE GLYCOL MONOETHYL ETHER) (OXITOL	110805																3.0		
718	3-HYDROXYNONANOIC ACID	33796871																3.0		
719	P-BROMOBENZOIC ACID	586765																3.0		
720	2,4-DIBROMOBENZOIC ACID	611007																3.0		

(Continued)

TABLE 10. (Continued)

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COMBINED CONCENTRATE REPORT(PART I.A)

RELATIVE SIZE

	COMMON NAME	CAS NO.	V1C	X1C	L2P	L2H	L2N	L2D	C3C	C1P	G1H	C1N	G2N	R1C	R2C	E1C	D2N	B2C	B1H	B1N
721	2,4,6-TRIBROMOPHENOL,	2001																3.0		
722	4-PHENYL-4-OXO-BUTYRIC ACID	3333																3.0		
723	4(2,5-XYLYL)BUTYRIC ACID	127																3.0		
724	2,5-DI(CHLOROMETHYL)-3-ETHYL BENZOIC ACI	128																3.0		
725	N-ETHYL-4-METHYL-2-PENTANEAMINE	42966643																3.0		
726	O-CRESYL ACETATE	533186																3.0		
727	5-HEXEN-2-OL	54774275																3.0		
728	DIHYDRO-5-METHYL-2(3H)-FURANONE	108292																	3.0	
729	2,2-DIETHYLPROPYLENE GLYCOL	115764																	3.0	
730	4-ETHYLPHENOL	123079																	3.0	
731	ALPHA-OXOBENZENEACETIC ACID, ETHYL ESTER	1603798																	3.0	
732	3-DICHLOPOMETHYL-4,6-DI-T-BUTYL-0-BENZOQ	264																	3.0	
733	2,2,6-TRIMETHYL-1,4-CYCLOHEXANEDIONE	20547993																	3.0	
734	CYCLOPENTANE CARBOXYLIC ACID, VINYL ESTE	16523061																	3.0	
735	2,2-DICHLOROBUTYRIC ACID	13023002																		3.0
736	2,3,3-TRICHLORO-2-PROPENOIC ACID	2257354																		3.0
737	2-METHOXY-2-HEXENOIC ACID	144																		3.0
738	2-HEPTENOL	33467764																		3.0
739	1-(2-METHOXY-1-METHYLETHOXY)-2-PROPANOL	20324327												1.0				2.6	
740	ABIETIC ACID	624	0.0															2.0*		
741	2,4,6-TRICHLOROANILINE	634935	-1.0						1.0*			1.0*			2.0*			0.0*		
742	METHYL PENTADECANOATE	7132641	1.0		2.0*															
743	AMYLENE DICHLORIDE	907459		2.0											0.0*					
744	X+ACENAPHTHALENE	83329		2.0			0.0*				1.0*				1.0*		0.0*		0.0*	0.0*
745	DIETHYL CARBINOL	584021		2.0																
746	2-METHYLFURAN	534225		2.0																
747	1-(2-PROPENYLOXY)HEPTANE	16519247		2.0																
748	3-METHYL-4-(2,5-XYLYL) BUTANOIC ACID	30275764			2.0															
749	XCARVACROL	499752			2.0															
750	XSO-XYLENE	95476			2.0								1.0							
751	TETRALIN	119642			2.0															
752	1-METHYL-7-ISOPROPYL NAPHTHALENE	490653			2.0		1.0					2.0								
753	X+9H-FLUORENE	86737			1.0		1.0		1.0					2.0	2.0				2.0	
754	1,2,3,4-TETRAMETHYL BENZENE	488233			2.0															
755	2-METHYL BIPHENYL	643583			2.0															
756	METHYLISOBUTYL BENZENE	108			2.0										0.0					
757	C5 BENZENE	118			2.0															
758	C6-BENZENE	250			2.0															
759	C5 BENZENE	119			2.0															
760	ETHYL TRIMETHYL BENZENE	113			2.0															
761	DIETHYL TOLUENE	108			2.0															
762	DIMETHYL ISOPROPYL BENZENE	104			2.0															
763	DIMETHYL ISOPROPYL BENZENE	105			2.0															
764	DIMETHYL INDAN	617			2.0															
765	5-METHYL TETRALIN	2809645			2.0					2.0										

(Continued)

TABLE 10. (Continued)

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COMBINED CONCENTRATE REPORT(PART I.A)

	COMMON NAME	CAS NO.	RELATIVE SIZE																	
			V1C	X1C	L2P	L2M	L2N	L2D	C3C	C1P	C1M	C1N	C2N	R1C	R2C	E1C	D2N	D2C	B1M	B1N
766	2-PHENYL UNDECANE	4536883			2.0												0.0			
767	C3 NAPHTHALENE	315			2.0		1.0		1.0											
768	TRIMETHYLNAPHTHALENE	316			2.0		2.0		1.0											
769	P-ETHYL TOLUENE	622968			2.0					2.0										
770	2,6-DIMETHYLSTYRENE	2039909			2.0															
771	INDAN	496117			2.0															
772	1,3-DIETHYL BENZENE	141935			2.0			0.0							0.0					
773	2-PHENYLHEXANE	6031023			2.0															
774	1,2,3,4-TETRAHYDRO-4,9-DIMETHYL ACRIDINE	55030654			2.0															
775	%*+CHRYSENE	218019			2.0															
776	(2,2-DIMETHYLBUTYL) BENZENE	28080866			2.0															
777	1,4-DIETHYL-2,3,5,6-TETRAMETHYL BENZENE	33962139			2.0															
778	1-BUTYLNAPHTHALENE	1634099			2.0		2.0													
779	1,5,7-TRIMETHYL INDAN	54340884			2.0															
780	1,1,4,7,7,8-HEXAMETHYL-S-HYDRINDACENE	17465586			2.0															
781	BENZOFLUORANTHENE	203123			2.0															
782	DIPHENYLMETHANE	101815			2.0															
783	SEC-BUTYL BENZENE	135988			1.0					2.0										
784	%2,3-DIMETHYLNAPHTHALENE	581408			2.0						1.0									
785	TRIMETHYLNAPHTHALENE	317			2.0				1.0						1.0					
786	C3 NAPHTHALENE	318			2.0															
787	2-METHYL FLUORENE	1430973			2.0															
788	%2-METHYL ANTHRACENE	613127			2.0															
789	1-TERT-BUTYLNAPHTHALENE	17085915			1.0		2.0													
790	%MENTHOL	89781			2.0															
791	%N-BUTYLETHER	142961			2.0															
792	3,3,5-TRIMETHYCYCLOHEXANONE	873949			2.0															
793	%THUJYL ALCOHOL	513235			2.0															
794	TERPENYL ACETATE	4821049			2.0															
795	DIACETYLBENEZENE	1009616			2.0															
796	HEX-3-ENE-2,5-DIOL	7319235			2.0															
797	4,4*-DIMETHOXYSTILBENE	4705344			2.0															
798	O-TERT-BUTYLPHENOL	88186			2.0															
799	METHYL ANTEISOHEPTADECANOATE	2490495			2.0															
800	2-METHYL-1-PENTEN-3-OL	2088075				1.0						2.0								
801	METHOXYNAPHTHALENE	2216695				2.0														
802	*2-METHYL STYRENE	611154				1.0	1.0	1.0	1.0	1.0	2.0	1.0	1.0		1.0					
803	TETRAPROPYLENE GLYCOL METHYL ETHER	20324349				2.0														
804	M-METHOXYPHENYL ACETATE	1024				2.0														
805	3,3,4-TRIMETHYLDECANE	49622186				2.0														
806	N-TRIETHYLENE GLYCOL, MONOETHYL ETHER	112505				2.0		2.0												1.0
807	N-METHYL SACCHARIN	15448994					2.0													
808	2-KETO-3-METHYL VALERIC ACID	1460340					2.0													
809	TRANS-3-HEPTENOIC ACID	29901857					2.0													
810	PENTACHLOROPYRIDINE	2176627					1.0					2.0	2.0							

(Continued)

TABLE 10. (Continued)

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COMBINED CONCENTRATE REPORT(PART I.A)

	COMMON NAME	CAS NO.	RELATIVE SIZE																	
			V1C	X1C	L2P	L2M	L2N	L2D	C3C	C1P	C1M	C1N	C2N	R1C	R2C	E1C	D2N	B2C	B1M	B1N
811	~~PENTADECANE~~	~~629629~~					~~2.0~~													
812	~~HEPTADECANE~~	~~629787~~					~~2.0~~													
813	~~NONADECANE~~	~~629925~~					~~2.0~~													
814	1-ISOBUTYLNAPHTHALENE	16727916					2.0													
815	1,1,2-TRIMETHYL-3-PHENYL INDAN	33508020					2.0													
816	~~OCTADECANE~~	~~593453~~					~~2.0~~													
817	1,2,3-TRIMETHYL-1-PHENYL INDAN (STERIOIS	33603393					2.0													
818	1,2,3-TRIMETHYL-1-PHENYL INDAN (STEREOIS	33611164					2.0													
819	~~HEXACOSANE~~	~~630013~~					~~2.0~~													
820	~~HEPTACOSANE~~	~~593497~~					~~3.0~~													
821	%*+$HEXACHLOROBENZENE	118741					1.0					2.0	1.0		1.0				1.0	
822	3,4,4-TRIMETHYL-2-CYCLOHEXEN-1-ONE	17299411					2.0													
823	~~1-UNDECYNE~~	~~100430~~					~~2.0~~													
824	~~5-UNDECYNE~~	~~2243903~~					~~2.0~~													
825	%M-ACETOTOLUIDE	537928					2.0													
826	NONYL PHENOL ISOMER	510					2.0													
827	%GLYCIDYL PHENYL ETHER	122601					2.0													
828	4,7-DIMETHYLBENZOFURAN	28715266						0.0				2.0								
829	(1,2-DICHLOROETHYL)BENZENE	1074119						1.0				2.0					1.0			
830	2-CYCLOHEXENOL	822673						2.0				2.0	2.0					2.0		
831	%CLOFIBRATE	637070						2.0												
832	%ETHYLENE GLYCOL	107211							2.0											
833	1,3,5-TRICHLORO-2-METHOXYBENZENE	87401							2.0					2.0						
834	%*+$P-DICHLOROBENZENE	106467							1.0			2.0			1.0					
835	METHYL 4-BUTOXYBUTYRATE	29006062							2.0											
836	*TRI-M-CRESYLPHOSPHATE	563042							2.0											
837	3-METHYL ADIPIC ACID	61898586								2.0										
838	CYMENE (ISOMER UNKNOWN)	208								2.0										
839	CYMENE (ISOMER UNKNOWN)	209								2.0										
840	%*+$1,2,4-TRICHLOROBENZENE	120821								2.0		1.0			1.0					
841	1,2,4-TRIMETHYL ETHYL BENZENE	54120626								2.0										
842	2,4,5-TRIMETHYLETHYL BENZENE	17851273								2.0										
843	DIETHYL TOLUENE	25550134								2.0										
844	2,4,6-COLLIDINE	108758									2.0			2.0	2.0					
845	BENZONITRILE	100470									2.0									
846	2-AMINO-5-PICOLINE	1603414									2.0									
847	TRANS-2-ETHYL-3-PROPYLOXIRANE	56052950										2.0								
848	P-METHYLANISOLE	104938										2.0								
849	2,3,4-TRIMETHYLOXETANE	53778613										2.0								
850	2,5-DIMETHYL THF	1003389										2.0								
851	4-BROMO-3-PHENYLSYDNONE	13183090										2.0								
852	3,8-DIMETHYL-5-ISOPROPYL-1,2-NAPHTHOQUIN	5574345										2.0								
853	CHLOROIODOMETHANE	593715										2.0								
854	1-METHYL-4-(1-METHYLETHENYL)-CYCLOHEXENE	138863										2.0								
855	1-(2-BROMOETHYL)-4-CHLOROBENZENE	6529539										2.0					0.0			

(Continued)

TABLE 10. (COntinued)

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COMBINED CONCENTRATE REPORT(PART I.A)

	COMMON NAME	CAS NO.	RELATIVE SIZE																	
			V1C	X1C	L2P	L2M	L2N	L2D	C3C	C1P	C1M	C1N	C2N	R1C	R2C	E1C	D2N	B2C	B1M	B1N
856	3,4,5,6-TETRAMETHYLPHENANTHRENE	7343066										2.0			1.0					
857	2,4,5,7-TETRAMETHYLPHENANTHRENE	7396385										2.0								
858	(2-BROMOCYCLOPROPYL)BENZENE	36617024										2.0								
859	OCTAHYDROAZOCINE	1121922										2.0								
860	PIPERIDONE	89816										2.0								
861	COUMARONE	271896										2.0								
862	P-TOLYL ACRYLIC ACID	1866393										2.0								
863	N-HEXYLBUTANAMIDE	10264172										2.0								
864	4H-PYRAN-4-ONE	108974										2.0								
865	5-DECANONE	820291										2.0								
866	3,3-DIMETHYL-2-HEXANONE	26118387										2.0								
867	4-METHYLHEXANAL	41065978										2.0							2.0	
868	~~%DIMETHYL SULFATE~~	~~77781~~											~~2.0~~							
869	%GUAIACOL	90051											2.0							
870	1-VALERYLPYRROLIDINE	4419572											2.0							
871	1-ETHYL-2,5-PYRROLIDINEDIONE	2314785											2.0							
872	METHYL CAPROATE	106707											2.0							
873	1-ACETYLPIPERIDINE	618428											2.0							
874	CONIINE	458888											2.0							
875	HEPTYL ACETATE	112061											2.0							
876	ETHYL BUTYL KETONE	106354											2.0		1.2					
877	DIPROPYL CARBINOL	589559											2.0						2.0	
878	HEPTYL ALCOHOL	111706											2.0							
879	TRANS-2-METHYLCYCLOPENTANOL	25144041											2.0							
880	~~PHOSPHORIC ACID~~	~~2000~~												~~2.0~~						
881	%PHENYL ETHER	101848												1.0	2.0					
882	2,4,5-TRICHLOROANILINE	636306												2.0						
883	1,5-DIPHENYL-3-PENTANONE	5396918												2.0						
884	4-PHENYLBICYCLOHEXYL	20273272												2.0	1.0					
885	OCTAHYDROPHENANTHRENE CARBOXALDEHYDE	24035505												2.0	2.0					
886	2,3-LUTIDENE	583619												2.0	2.0					
887	%N,4-DIMETHYLBENZENESULFONAMIDE	640619												2.0						
888	4-METHYLPHTHALIC ACID	4316238													2.0					
889	4,6-DIMETHYLNONANOIC ACID	19943716													2.0					
890	%O-CHLORONITROBENZENE	88733													2.0					
891	DIMETHYLFLUORENE	4612639													2.0					
892	4-METHYLPHENANTHRENE	832644													2.0					
893	1,2,3,4-TETRACHLOROBUTANE	3405680													2.0					
894	%3-METHYLPHENANTHRENE	832713													2.0					
895	%N-AMYL ALCOHOL	71410													2.0					
896	%METHYLAL	109875													2.0					2.0
897	4-PENTEN-2-OL	625310													2.0					
898	2,2-DIMETHYL-1,3-CYCLOPENTANEDIONE	3883587													2.0					
899	5-DODECANONE	19780100													2.0					
900	%QUINOLINE	91225													2.0				1.0	

(Continued)

TABLE 10. (COntinued)

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COMBINED CONCENTRATE REPORT(PART I.A)

	COMMON NAME	CAS NO.	RELATIVE SIZE																	
			V1C	X1C	L2P	L2M	L2N	L2D	C3C	C1P	C1M	C1N	C2N	R1C	R2C	E1C	O2N	O2C	O1M	O1N
901	TETRAPROPYLENE GLYCOL	1376																		
902	N-ETHYL-2-BENZOTHIAZOLAMINE	28291692													2.0					
903	N,N-DIMETHYLBENZYLAMINE	103833													2.0					
904	DIMETHYLCYCLOHEXANE DIONE	126818													2.0					
905	2,2,4-TRIMETHYL-1,3-PENTANEDIOL	144194													2.0				2.0	
906	METHYL LAURATE	111820													2.0					
907	ETHYL MYRISTATE	124061													2.0					
908	6-METHOXY-2-HEXANONE	29006006													2.0					
909	6-METHYL-2-HEPTANONE	928687														2.0				
910	1,2-DIAZABICYCLO(2.2.2.)OCTAN-3-ONE	1632264														2.0				
911	2-METHOXY-10-UNDECENOIC ACID	214														2.0				
912	5,6,7,7A-TETRAHYDRO-4,4,7A-TRIMETHYL-2(4	15356748															2.0			
913	1-PROPOXY-2-PROPANOL	1569013															2.0			
914	2-ETHYLHEPTANOIC ACID	3274291																2.0		
915	5-METHYL-5-ETHYL-2,4-OXAZOLIDINEDIONE	115673																2.0		
916	X3,5-DICHLOROPHENOL	591355																2.0		
917	BROMOCHLOROBENZOIC ACID	25638146																2.0		
918	16-HYDROXY PALMITIC ACID	506138																2.0		
919	OCTAHYDRO-1,4A-DIMETHYL-1-PHENANTHRENE C	3650042																2.0		
920	4,6-DIMETHYL OCTANOIC ACID	2553960																2.0		
921	5-METHYL-2-HEPTANONE	18217124																2.0		
922	2-METHYLENEBUTYRIC ACID	3586581																2.0	1.0	
923	P-AMINOBENZENE-T-BUTYRIC ACID	15118602																	2.0	
924	5-ETHENYL TETRAHYDRO-.ALPHA.,.ALPHA.,5-T	5989333																	2.0	
925	6-METHYL-3,5-HEPTADIEN-2-ONE	16647044																	2.0	2.0
926	TRIMETHYL-6-VINYLTETRAHYDROPYRAN-3-OL	14049117																	2.0	
927	2-METHYL-2-HEPTEN-4-ONE	22319248																	2.0	2.0
928	3,4-DIMETHYL-2,5-FURANDIONE	766392																	2.0	
929	XETHYL CARBONATE	105588																	2.0	
930	4,4-DICHLOROBUTENOIC ACID	16502888																	2.0	
931	BARBITAL	2510721																		2.0
932	2-BROMO-1,2-DICHLOROPROPANE	17759885																		2.0
933	METHYL DICHLOROACETATE	116541																		2.0
934	3-OCTEN-2-ONE	1669449																		2.0
935	2,3,4-TRIMETHYL-2-CYCLOPENTEN-1-ONE	28790865																		2.0
936	5,5-DIMETHYLFURANONE	137																		2.0
937	5-HEPTEN-2-ONE	6714007																		2.0
938	N-METHYL-2-PIPERIDINONE	931204																		2.0
939	3,4-DIMETHYL-3-PENTEN-2-ONE	684946																		2.0
940	METHYL-9,11-OCTADECADIENOATE	13038476	1.0																	2.0
941	N-BENZOYL-L-ALANINE, METHYL ESTER	7244679	1.0																	
942	9,12-OCTADECADIENOIC ACID	60333	1.0																	
943	1-HEXANOL	111273	0.2		1.0 *															
944	1,1,2,3-TETRACHLOROPROPANE	18495302		1.0																
945	6-PHENYL-2-HEXANONE	14171892		1.0													1.0*			
																		1.0*		

(Continued)

TABLE 10. (Continued)

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COMBINED CONCENTRATE REPORT(PART I.A)

	COMMON NAME	CAS NO.	RELATIVE SIZE																	
			VLC	X1C	L2P	L2M	L2N	L2D	C3C	C1P	C1M	C1N	C2N	R1C	R2C	E1C	D2N	B2C	B1M	B1N
946	3-PENTEN-2-ONE	625332		1.0																
947	3-METHYL-2-BUTEN-1-OL	556821		1.0																
948	4,4,5-TRIMETHYL-1,3-DIOXAN-1-OL	54063148		1.0																
949	TETRAMETHYL BIPHENYL	4920950			1.0				1.0											
950	HEXAMETHYL BIPHENYL	56667017			1.0															
951	$N-PROPYL BENZENE	103651			1.0															
952	4,5,7-TRIMETHYLINDAN	6682060			1.0															
953	1,4-DIMETHYL-2-ISOBUTYL BENZENE	55669880			1.0															
954	PHENYLCYCLOHEXANE	827521			1.0															
955	1-ETHYLNAPHTHALENE	1127760			1.0															
956	1,3,5-TRI-TERT-BUTYL BENZENE	1460022			1.0				1.0											
957	1,1,4,5,5,8-HEXAMETHYL-S-HYDRINDALENE	17465597			1.0															
958	NEOPENTYL BENZENE	1007267			1.0															
959	(1,2,2-TRIMETHYLPROPYL) BENZENE	19262205			1.0															
960	1-METHYL-2-(1-ETHYLPROPYL) BENZENE	54410741			1.0															
961	(2-ETHYLBUTYL) BENZENE	19219853			1.0															
962	9-ETHYL PHENANTHRENE	3674757			1.0										1.0					
963	1,6-DIMETHYL INDAN	17059482			1.0															
964	1,2-DIMETHYL INDAN	17057828			1.0															
965	1,4,7-TRIMETHYL INDAN	54340873			1.0															
966	1,2,4-TRIMETHYL PHENANTHRENE	23189642			1.0															
967	2,9,10-TRIMETHYL ANTHRACENE	63018940			1.0															
968	OCTYL BENZENE	2189608			1.0															
969	1,1,3-TRIMETHYL INDAN	2613765			1.0															
970	%9-METHYL ANTHRACENE	779022			1.0															
971	ISOBUTYL BENZENE	538932			1.0															
972	META-CYMENE (M-ISOPROPYL TOLUENE)	535773			1.0						1.0									
973	DIMETHYL ETHYL BENZENE	202			1.0															
974	1,8-DIMETHYL TETRALIN	25419334			1.0															
975	1,2-DIMETHYL NAPHTHALENE	573988			1.0															
976	METHYL ACENAPHTHENE (ISOMER UNKNOWN)	58548302			1.0															
977	%DI-N-BUTYLNITROSAMINE	924163			1.0															
978	3,3,3-TRICHLOROPROPENE	2233003				1.0														
979	TERT-BUTYLBENZENE	98066				1.0					1.0									
980	4,6-DIMETHYL PYRIMIDINE	1558174				1.0														
981	2,3-DIMETHYL PYRAZINE	5910894				1.0														
982	PYRAZOLE	288131				1.0														
983	N-PROPYLNAPHTHALENE	325					1.0	1.0												
984	TRIMETHYLNAPHTHALENE	319					1.0	1.0												
985	METHYL NONADECANOATE	1731948					1.0											1.0		
986	~~TRIDECANE~~	~~629505~~					~~1.0~~	~~1.0~~												
987	~~N-TETRADECANE~~	~~629594~~					~~1.0~~													
988	%CINNAMYL ALCOHOL	104541					1.0													
989	2-T-BUTYL NAPHTHALENE	2876359					1.0													
990	2-METHYL-1-PROPYLNAPHTHALENE	54774899					1.0													

(Continued)

TABLE 10. (Continued)

COMBINED CONCENTRATE REPORT(PART I.A)

	COMMON NAME	CAS NO.	RELATIVE SIZE V1C	X1C	L2P	L2M	L2N	L2D	C3C	C1P	C1N	C1N	C2N	R1C	R2C	E1C	D2N	B2C	B1M	B1M
991	NONYL PHENOL ISOMER	511					1.0													
992	%INDENE	95136					1.0													
993	CHLOROVINYLBENZENE	622253						0.0				1.0								
994	GAMMA METHYLBENZENEBUTANOIC ACID, METHYL	24306238						1.0												
995	2-METHYLBENZAMIDE	6886						1.0												
996	%*M-NITROANILINE	99092						1.0												
997	4-TERT-BUTYL-2-METHYLPHENOL	98271						1.0												
998	1-METHYL-3-PROPYL BENZENE	1074437							1.0											
999	3-METHYL-3-HEXANOL	597966							1.0											
1000	1-ALLYLBENZENE	637503							1.0											
1001	DIETHYLMETHYLVINYLSILANE	18292290							1.0											
1002	%M-CHLORONITROBENZENE	121733							1.0											
1003	2-PHENYL-1,4-CYCLOHEXADIENE	1370521							1.0											
1004	1,4-DIMETHYL-5-OCTYLNAPHTHALENE	55000538							1.0		1.0									
1005	1-ALLYLNAPHTHALENE	2489863							1.0			1.0								
1006	3,4'-DIMETHYL-1,1'-BIPHENYL	7383906							1.0											
1007	ETHYLBENZYL BENZENE (ISOMER UNKNOWN)	425504541							1.0											
1008	~~PENTATRIACONTANE~~	~~630079~~							~~1.0~~											
1009	~~DI-P-TOLYLMETHANE~~	~~4957146~~							~~1.0~~											
1010	DIMETHYLDIPHENYLMETHANE	13540562							1.0											
1011	AMYL BENZENE	538681								1.0										
1012	5-METHYL INDAN	874351								1.0		1.0								
1013	1-METHYL TETRALIN	1559815								1.0	1.0									
1014	%*TRIPHENYL PHOSPHATE	115866								1.0					1.0					
1015	PARA-METHOXYSTILBENE	1142150								1.0										
1016	1,2,4-TRITERTIARY BENZENE	1459116									1.0									
1017	*P-CHLOROACETOPHENONE	99912									1.0									
1018	3-METHYL-2-HEXANOL	2313657										1.0								
1019	P-ETHYL-ISOPROPYLBENZENE	4218488										1.0								
1020	2,6-DI-TERT-BUTYL TETRALIN	42981760										1.0								
1021	1,1,3-TRICHLORO-1-PROPENE	2567148										1.0								
1022	1-BROMO-2-CHLOROCYCLOPENTANE	14376820										1.0								
1023	7-ETHYLQUINOLINE	7661474										1.0								
1024	BETA,BETA-DIMETHYL HISTAMINE	21150816										1.0								
1025	3-CYCLOHEXYL-4-PENTEN-2-ONE	55702540										1.0								
1026	~~HEPTANE~~	~~142825~~										~~1.0~~								
1027	DIISOBUTYL KETONE	108838										1.0								
1028	5-METHYL-5-PHENYL-2-HEXANONE	14128611										1.0								
1029	4-DECANONE	624168										1.0								
1030	6-METHYL-2-PHENYLQUINOLINE	27356463											1.0							
1031	HEXAMETHYLENE ACETAMIDE	5809416											1.0							
1032	4-METHYL-3-HEXANOL	615292											1.0							
1033	HEXYL BUTYRATE	2639636											1.0							
1034	%*(2,4,5-TRICHLOROPHENOXY)ACETIC ACID	93765													1.0					
1035	*TRICHLOROBIPHENYL	25323686												1.0						

(Continued)

TABLE 10. (Continued)

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COMBINED CONCENTRATE REPORT(PART I.A)

	COMMON NAME	CAS NO.	RELATIVE SIZE																	
			V1C	K1C	L2P	L2M	L2N	L2D	C3C	C1P	C1N	C1N	C2N	R1C	R2C	E1C	D2N	B2C	B1M	B1N
1036	2,3,6-TRIMETHYLHEPTANE	4032933												1.0						
1037	+%*$LINDANE	58899													1.0					
1038	%*O-CHLOROTOLUENE	95498													1.0	1.0				
1039	%*+$HEPTACHLOR	76448													1.0					
1040	*$TETRACHLOROBIPHENYL	26914330													1.0					
1041	*+$PENTACHLOROBIPHENYL + OTHER PCBS	000													1.0					
1042	*$HEXACHLOROBIPHENYL	26601649													1.0					
1043	%+$DDE	72559													1.0					
1044	%*+$DDT	50293													1.0					
1045	DIBENZOTHIOPHENE	132650													1.0					
1046	4-METHYLDIBENZOTHIOPHENE	7372885													1.0					
1047	%ETHYLENE TETRACHLORIDE	127184													1.0					
1048	O-ETHYLSTYRENE	7564630													1.0					
1049	1,1,2,3,3-PENTACHLOROPROPANE	15104617													1.0					
1050	1,6-DICHLORO-1,5-CYCLOOCTADIENE	29480420													1.0					
1051	2-ETHYL-1,1-BIPHENYL	1812517													1.0					
1052	1-METHYLFLUORENE	1730376													1.0					
1053	METHYLBENZACRIDINE	3519877													1.0					
1054	3-HYDROXY-3-METHYL-2-BUTANONE	115220													1.0					
1055	%2,4-LUTIDINE	108474													1.0					
1056	2,5-LUTIDINE	589935													1.0					
1057	2,4,5-COLLIDINE	1122390													1.0					
1058	4-ETHYL-2,6-DIMETHYL PYRIDINE	36917369													1.0					
1059	2,3,5-COLLIDINE	695987													1.0					
1060	3-ETHYL-5-METHYLPYRIDINE	3999788													1.0					
1061	2,3,6-TRIMETHYLPYRIDINE	1462846													1.0					
1062	N,N-DIETHYLANILINE	91667													1.0					
1063	3-DODECANONE	1534276													1.0					
1064	4-ACETYLMORPHOLINE	1696204													1.0					1.0
1065	%QUINAIDINE	91634													1.0					
1066	2,3,4-TRIMETHYLQUINOLINE	2437721													1.0					
1067	TRIMETHYLQUINONE	1364													1.0					
1068	HEXANEDIOIC ACID, DIHEXYL ESTER	1759													1.0					
1069	%*P-NITRO PHENOL	100027														1.0				
1070	3-CHLORO-2-BUTANOL	563840														1.0				
1071	7-OXO-OCTANOIC ACID	14112982															1.0			
1072	3-METHYLPIPERIDINE-2,6-DIONE	29553513															1.0			
1073	5-PROPYLDIHYDRO-2-FURANONE	105215															1.0			
1074	3A,7A-DIMETHYL OCTAHYDRO-4-ISOBENZOFURAN	54382580															1.0			
1075	~~UNDECANE~~	~~1120214~~															~~1.0~~			
1076	3-METHYL-3-OCTANOL	5340363																1.0		
1077	BROMODICHLOROANILINE	739																1.0		
1078	HEPTYLPROPIONATE	2216811																	1.0	
1079	ACETAMIDE	60355																	1.0	
1080	%CHLOROACETIC ACID	79118																		1.0

(Continued)

TABLE 10. (Continued)

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COMBINED CONCENTRATE REPORT(PART I.A)

	COMMON NAME	CAS NO.	RELATIVE SIZE V1C	X1C	L2P	L2M	L2N	L2D	C3C	C1P	C1M	C1N	C2N	R1C	R2C	E1C	D2N	B2C	B1M	B1N
1081	4-CHLOROCROTONIC ACID	16197903																		1.0
1082	*2,4-DICHLORONAPHTHALENE	2198756																		1.0
1083	SEC-ISOAMYL ALCOHOL	598754																		1.0
1084	5-(ACETYLOXY)-2-PENTANONE	5185977																		1.0
1085	3,4,5-TRIMETHYL-2-CYCLOPENTEN-1-ONE	55683211																		1.0
1086	DIETHYLENE GLYCOL, MONOMETHYL ETHER	111773																		1.0
1087	N-BUTYLAMINE	109739																		1.0
1088	2,4-DIISOPROPYLPHENOL	2934056																		1.0
1089	METHYLOCTADEC-10-ENOATE	13038454	0.0																	
1090	METHYL ISOPALMITATE	5129602	0.0																	
1091	X+BDIHEXYL PHTHALATE	84753	0.0																	
1092	3-BROMOPENTANE	1809105						0.0												
1093	PHENYLPROPYL ETHER	622855						0.0												
1094	BENZOTHIOPHENE	95158						0.0												
1095	PHENALENE	203805						0.0												
1096	4-ETHYLSTYRENE	3454077						0.0												
1097	3,3-DIMETHYL-2(3H)-FURANONE	13524760						0.0												
1098	FLUOROIODOBENZENE (ISOMER UNKNOWN)	1111																		
1099	3-METHYL-2-FURANONE	22122367													0.0					
1100	1,4,5-TRIMETHYL NAPHTHALENE	2131411															0.0			
1101	3-METHOXY-3-METHYL-2-BUTANONE	36687986															0.0			
1102	DIBROMOPHENOL	546	-1.0														0.0			
1103	1H-IMIDAZOLE-2-CARBOXALDEHYDE	10111087	-1.0																	
1104	2-(4-METHYL-3-CYCLOHEXENYL)ISOPROPANOL	10482561	-1.0																	
1105	1,2-CYCLOHEXANEDIOL	931179	-1.0																	
1106	METHYL HEPTADECANOATE	1731936	-1.0																	
1107	BUTYL THIAZOLE	6086222	-1.0																	

* RS ENTRIES LABELED WITH AN ASTERISK ARE PROBABLY ATTRIBUTABLE TO THE BLANK ASSOCIATED WITH CONCENTRATE GENERATION. SEE DISCUSSION IN TEXT OF VOLUME 1.

TABLE 11. COMBINED LISTING OF IDENTIFIED COMPOUNDS FOUND IN DW AND AWT CONCENTRATED

FINAL REPORT (PART I)

RELATIVE SIZE AND CONCENTRATE WHERE DETECTED

	COMMON NAME	*	V1G	V1X	T2B	T1C	T1X	T1Y	T4C	T4X	M2C	N2C	P2C	P2X	O2C	O2X	S2C	S2X	L2N	O3C	C1M	C1N	C2N	R1C	R2C	E1C	D2N	B2C	B3C
1	CLOFIBRIC ACID †					5		5	5		6	5	6		5				7		6	7	7			4	3	3	3
2	X*$DI-N-BUTYLPHTHALATE		2	1	3	5		5		1*	9	8	8		4*		2*	3*	6*	9		3*	4*	8	7	7	5*	8	6*
3	2-(2-BUTOXYETHOXY)ETHANOL (A DIETHYLE					3	4		4	3	6	6		5	5	2	3	4		9	5			6	5	6		5	1
4	DIETHYLENE GLYCOL, 4-METHOXYBUTYL BUTYL																			9									
5	DIETHYLENE GLYCOL, 2-METHOXYBUTYL BUTYL																			9									
6	X*$DIOCTYLPHTHALATE			3	2			5*				2*		3*							6			8	7			2	
7	1-(2-BUTOXYETHOXY) ETHANOL			2					8				2		4		2	1*	3	8	3	7		5	5	5			
8	XTRIS-B-CHLOROETHYL PHOSPHATE								3										3		8	4	5		5		3		3
9	X*NAPHTHALENE	a		5	1		5*		1	4*				8*	5	8*	2				6					1	1		
10	2-ETHYL-1,1-BIPHENYL	A		6						4*			2	8*	1	5*									1				
11	XPALMITIC ACID				3	7			5*	4*	8	6*	6*	2*	5*	2*	5	1*	5*		5*		5*	6*	7*			5*	5*
12	X1-BUTANOL						3				5	7		3				2	5		2			6	6	4	5	6	4
13	2-HYDROXY-2-METHYLPROPANOIC ACID							7			2																		2
14	2-ETHYL-3-METHYLMALEIC ACID					7	5		6	5	6	7	5		7	5	4	4			5	3			5		4	4	6
15	1-(1-METHYLPROPOXY)-2-PROPANOL					7									1														
16	TRIETHYLENE GLYCOL N-BUTYL ETHER		1																5*	7				4*					
17	DIOCTYL ADIPATE		0	0			2*	5*	0*	3*	4*		4*		2*	1*			3*		4*				7	4*		7	
18	XBIS(2-ETHYLHEXYL) ADIPATE		0		3	4*					4*	3*			4*	4*			2*		5	3*		7					5
19	X$1,1,2,2-TETRACHLOROETHANE				5	5*	4*		3*		2*						8*	1*	3*	3*	7*	6*	6*		6*			4*	0*
20	DIHEXYLADIPATE				1			4																7	7				9
21	XMETHYL BENZOATE				7			5																					
22	XSTEARIC ACID					6			4			4			5		5		5		4			6	7		3	4	4
23	DIETHYLENE GLYCOL, BUTYL ETHER							1				2			4		8		2			4	4		7				
24	DIISOOCTYLPHTHALATE									5															7				
25	$BUTYL-BUTOXY ETHYL PHTHALATE																		7								2		
26	$BUTYL METHYL PHTHALATE																			4			7	4	4	3	1	4	
27	TRIETHYLENE GLYCOL, TERT-BUTYL ETHER																			7									
28	XCYCLOHEXANOL				5	5*	3		4*		7	7	6		9*		5		2*						4*		2*		4*
29	XMONOBUTYL PHTHALATE				1							7	7											6	6	3*	5	5	3*
30	1,2 5,6-BIS-O-ISOPROPYLIDENE-BETA-D-TALO												7		6														
31	1,2 4,5-DI-O-ISOPROPYLIDENE-ALPHA-D-FRUC												7												5				
32	2,3-DIMETHYLMALEIC ACID					6	4		6	5	6	7	6		6	5	4					5			4		4	4	5
33	PHTHALIC ANHYDRIDE											7													4		1		
34	XCYCLOHEXANONE					5			3		7	6	6		4		4	1	1								1		3
35	XBENZOIC ACID		0	4	5	5	6	6	5	4	7	6	6	5	5	6	4	5	5	2*	6	5	5	5	5	5	9	5	5
36	XMYRISTIC ACID		1		3	6			4*		7	5			4	2*	5		3*		4*		6*	6*	6*			9*	4*
37	PENTADECANOIC ACID		1		1	4*			3*		7	6*					3*		3*		3*			5*	6			3*	3*
38	X$DI-ISOBUTYLPHTHALATE		0	1		5					7	6	4							6		2*	3*	5	6	3*		5	
39	TRANS-2-METHYLCYCLOPENTANOL				2		4				7		5					3					2						
40	2-METHYLBUTYRIC ACID							3	4	4	7	4	5	3	4	5	4	2	3						4		1	3	5
41	2,2,4,4-TETRAMETHYL PENTANOIC ACID							3	3		7	4	4							4	4	3	5	3	3				3
42	XBUTYRIC ACID									5	7	3	3			3		3											
43	MARGARIC ACID										7	3*					3*							4*	5*		2*	3*	4*
44	1,2-PROPYLENE GLYCOL, DIMETHYL ETHER										7																		
45	2-HEPTENE										7																		

* SEE FOOTNOTE ON LAST PAGE

† THIS ENTRY APPEARS OUT OF ORDER. IT SHOULD APPEAR BETWEEN ENTRIES NO. 11 AND NO. 48.

(Continued)

TABLE 11. (Continued)

FINAL REPORT (PART I) PAGE 2

RELATIVE SIZE AND CONCENTRATE WHERE DETECTED

	COMMON NAME	V1C	V1X	T2B	T1C	T1X	T1Y	T4C	T4X	H2C	N2C	P2C	P2X	O2C	O2X	S2C	S2X	L2M	C3C	C1M	C1N	C2N	R1C	R2C	E1C	O2N	B2C	B3C
46	1,1-DICHLOROACETONE									7	6	5																
47	3-ETHYL-4-METHYL-2,5-FURANDIONE									7	6			6		2												
48	2-HYDROXY-3-METHYL-2-CYCLOPENTEN-1-ONE				4		5									6												
49	4-(HEXYLOXY)-1-BUTANOL											3		5		6												
50	6-BROMO-2-HEXANONE				4		6			5													3		3		4	
51	TRIPROPYLENE GLYCOL, METHYL ETHER							3	4	6			4					6		5	4	3	5					5
52	TRIPROPYLENE GLYCOL, METHYL ETHER							3	4	5		5	5					6		5	4	4	5	6				5
53	TRIPROPYLENE GLYCOL, METHYL ETHER							3	4	5		5	4					6		6	3							5
54	TRIPROPYLENE GLYCOL, METHYL ETHER							3		6		5	4					6										5
55	TRIPROPYLENE GLYCOL, METHYL ETHER											5						6										
56	XBROMODICHLOROMETHANE				1		6			3	2	1																
57	+ XBROMOFORM				2		6	1		5	4																	
58	4-METHYL-2-PENTANOL		3	6		6	6*					6	5*		5*			5	2*					1*			4	
59	X* +$2,4,5-TRICHLOROPHENOL	-2					6	4		1		5	0			2			5		2*	4		4			1	
60	X +$DIETHYL PHTHALATE	0		2	5	3	6	2*	4	5	5			4			1*	3*				2*	5	6	3*		6	
61	2,4,6-TRIBROMOPHENOL,						6																				3	
62	AMYLENE DICHLORIDE						6	3*		5	5	3*		3*		3	4							0*				
63	X9,10-ANTHRACENEDIONE						6																					
64	7,7-DIMETHYL-2-OXOBICYCLO(2.2.1)HEPTANE-						6																					
65	3-METHOXY-3-METHYL-2-BUTANONE						6			4	6					4										0		
66	4-HEXEN-3-ONE						6			4																		
67	XTRICHLOROPROPANE				6																							
68	1-METHOXY-2-PROPANOL			5	6	6						5	3	6	5		4	6								5		5
69	3-HEXANOL					6				6	5	3	3		3	1		5	2				4	2			2	2
70	XSALICYLIC ACID		1	1	6	3	4	4	5	4	4	5	4	4	4		3				5			6	3	2		5
71	XCAPRYLIC ACID			1	6		3	4	2		6	5	4	6	2	3	3	3		5		5	6	6		4	3	3
72	XPHENYLACETIC ACID				6	4	3	4	4	5	5	6	5	5	6	2	3	4					3	4		2	5	5
73	~~2,3-DIMETHYLMALEIC ACID~~ SEE NO. 32				6			6	6					6										4		4	4	6
74	XPELARGONIC ACID				6						4	4		4		3	2	3		5	2	5	6	6		4	4	2
75	1,3,5-TRIMETHYLCYANURIC ACID				6		5	4			5																	
76	XMETHYL BUTYLKETONE			5						5*		3*				2		6*		2*								
77	TRIPROPYLENE GLYCOL, METHYL ETHER								4									5					2	6				5
78	TRIPROPYLENE GLYCOL, METHYL ETHER																							6				5
79	TRIPROPYLENE GLYCOL, METHYL ETHER																							6				5
80	1-METHYLBUTYLALCOHOL			3	4					6	6	5		4		4							3					
81	3-PENTEN-2-OL						4	3*		6	6	6		5												1*		2*
82	2-BUTYL-N-BUTYRATE															3			6									
83	2-ETHYLHEXANOIC ACID	-1			5		3	6	3	4	6	6		4	3	4		4	5	6	2*	5	6	5		4	4	4
84	XCAPRIC ACID	0			4			4		5	6	5		4		4		4*		6			6	6	1*	3*	4*	
85	ELAIDIC ACID	2		1							4					3	1	4*						6				
86	P-PHENYLACETOPHENONE	0																						6	3*		4*	
87	PALMITOLEIC ACID	1						3*			5	5			2	4	2				4*			6				
88	X$DICYCLOHEXYL PHTHALATE	3	0					3*	1*						3*				3*						6		5*	5*
89	X +$BIS(2-ETHYLHEXYL) PHTHALATE	3			3*			5*		5*	5*	4*	3*	4*	4*			2*				1*	4*		2*	3*		5*
90	2,4-DICHLOROBENZOIC ACID		2			2					3					2					5							4

(Continued)

TABLE 11. (Continued)

FINAL REPORT (PART I)

RELATIVE SIZE AND CONCENTRATE WHERE DETECTED

	COMMON NAME	V1*G	V1X	T2B	T1G	T1X	T1V	T4G	T4X	N2C	N2G	P2G	P2X	O2G	O2X	S2G	S2X	L2M	C3C	C1M	C1W	C2W	R1C	R2G	E1G	O2W	B2C	B3G
91	%PHTHALIC ACID		0			1			3*	6	6	5	4	3*			2						6	6		3	5	3
92	N-BUTYLBENZENESULFONAMIDE		-1		2						5	4							6	5			4				3	5
93	%LAURIC ACID			4		4*		4*			6	3*	4*	4*	4*	5	4	3		5				6		3	5	3
94	%N-HEPTANOIC ACID				5	4	1	5	4	4	4	3	2	4		2	2			2	3	3	6	6		4	2	2
95	%ETHOSUXIMIDE					3		3	5						4		3	6						4		4	4	5
96	SUBERIC ACID					3			4		6		3	3	3							6	2	4		2	2	
97	O-CHLOROBENZOIC ACID						3						3			3	2		4		5	6				2	2	
98	2-KETOISOCAPROIC ACID						4		3				1							6								
99	%OLEIC ACID							4			6					3							4	6				5
100	5,5-DIMETHYLDIHYDROFURANONE							3				3		3		6	3			6								3
101	3-ETHYLHEXANOIC ACID									2								5						6				
102	2,4,5-TRIMETHYLBENZOIC ACID									3		4		4		3					4	6	1			1		
103	$N-BUTYL-ISOBUTYLPHTHALATE									6	4	6			3					3				6	3		6	
104	TRIPROPYLENE GLYCOL, METHYL ETHER (ISOME											1											5					6
105	DIOCTYL SEBACATE											3		4						6						3		6
106	TETRAHYDRO-2-METHYL-2-FURANOL													4													6	
107	%PHENOBARBITAL																	6		5	4			3	2			
108	2-ETHYLSUBERIC ACID																	6		4	4							
109	P-T-BUTYLPHENOXY ACETIC ACID																	4		6	5	5						
110	BUTYL BUTYRATE																							5				
111	3,5-DIMETHYLDIHYDROFURANONE																			6								1
112	P-TERT-BUTYLPHENOXYMETHYL ACETATE																			6						2		
113	3,5-DIMETHYL STYRENE																			6		1						
114	$METHYL ETHYL PHTHALATE																			6								
115	BUTYL METHOXYBUTYRATE																			6								
116	~~2-METHYLHEPTANE~~																			6								
117	%METHYL PROPYL KETONE																				6							
118	3,7-DIMETHYL-6-OCTENOIC ACID																						3	6				
119	TRIS(CHLOROPROPYL)PHOSPHATE																							6				
120	%4+-ETHYLACETOPHENONE	A	4				4*		3*				6*		4*		1*											
121	DEHYDROABIETIC ACID	1	0	2				4*			3*			6		2*		4*		2*			5	5	2*	3*	4	3*
122	3,4-DIETHYLBIPHENYL	A	5								2				6*													
123	1-METHYL INDENE	a	3						3*		1	1		6	2*													
124	%$TOLUENE			5					4			5			6		2	1*				4*			4*			
125	ISOVALERIC ACID				4		4	3	5	4	4	5	5	5	6		4	4									4	4
126	2,4-DIMETHYLBENZOIC ACID						3	3			2	4		3	6	4	2	2	2	4	2			3				
127	3-PENTEN-2-ONE													6		2												
128	HEXAHYDROTOLUENE													6														
129	%ACETOPHENONE	a	3	2	2		5*		4*	5	4	5	6*	3	5*	2	1	2		2	3	3				0		
130	6-METHYL-5-HEPTEN-2-ONE				3							4	6	3		2												5
131	2-ETHYL-1-HEXANOL	-1			4	5		4	5				6	3		5	3			3*	2*		3*	4			3*	4
132	2+-ETHYLACETOPHENONE	A	2										6*		5*													
133	M-TOLUIC ACID				4		3	3	3		5	6			2	4	3						4	4	2	2	3	
134	P-TOLUIC ACID				4		4	3		3		6	4			4	3			4		4	3	4	1	2	3	
135	+ISOPHORONE					3	1	3	3			6	4	2	4	1	2											

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FINAL REPORT (PART I)

RELATIVE SIZE AND CONCENTRATE WHERE DETECTED

	COMMON NAME	V1C	V1X	T2B	T1C	T1X	T1Y	T4C	T4X	M2C	N2C	P2C	P2X	O2C	O2X	S2C	S2X	L2M	C3C	C1M	C1N	C2N	R1C	R2C	E1C	D2N	B2C	B3C
136	2,6-DIMETHYLBENZOIC ACID										2	6		3		4	2				4	5						
137	1,5-HEPTADIENE-3,4-DIOL										5	6				5												
138	3-METHYL-2-BUTEN-1-OL									6				4		4												
139	BENZORESORCINOL										6					1												
140	%TRIBUTYL PHOSPHATE	1		1	3		5	4*		5*	6	5				3*							4*	5*	1*		5*	
141	%AZELAIC ACID		2	1	5	4		4	5*	4	6	5	4*	4	5*		2*					5	4*	5		3*	4*	3*
142	2-CYCLOPETEN-1-ONE										6																	
143	DICYANOHEXANE										6																	
144	%ATRAZINE										6			3														
145	1H-IMIDAZOLE-2-CARBOXALDEHYDE	-1								6		4			2													
146	%N-OCTANOL		3							6		5			1*								3	2				
147	CIS-2-METHYLCYCLOPENTANOL			4		5				6						0		4			2					1		1
148	%VALERIC ACID				4	1		3	5	6	5	3	3	4	4	3	2	4	3			2	2	4			3	4
149	%BICHLORACETIC ACID				5	3	4		4	6		3	3		2	3	4				5	5						
150	%TRIETHYL PHOSPHATE				3		4	4		6		4		2				2										3
151	5,6,7,7A-TETRAHYDRO-4,4,7A-TRIMETHYL-2(4				4	3			3	6	3	5		5	4											2		
152	3-METHYL-2-BUTENOIC ACID						2		3	6			1		3	3												
153	3-METHOXYPENTANE						3			6																		
154	6-METHYL-2-HEPTANONE							1		6		5		4		2									2			
155	%PROPYL ALCOHOL									6																		
156	2,2-DIETHYLPROPYLENE GLYCOL									6																		3
157	AMYL CHLORIDE									6		5																
158	3,5-DIMETHYLCYCLOHEXANOL									6	2			3		2												
159	1-METHYL-3-CYCLOHEXEN-1-OL									6																		
160	CYCLOHEXYL FORMATE									6		2				2											1	5
161	1,1,1-TRICHLORO-2-PROPANONE									6																		
162	%2-CHLORO-1,1-DIETHOXYETHANE						6																					
163	%DICAMBA		0		4			3	6		5		2			2	3											
164	%ISOBUTYRIC ACID								6				4							4		4						
165	2-METHYL-2,4-PENTANEDIOL								1																			5
166	2-METHYL-3-BUTEN-2-OL							3		5	5	5		4														
167	2-BUTOXYETHANOL				3	3		1	1				5		2		2	3		5	3	5		5	4	1		4
168	%BENZALDEHYDE		2	1	3	4	5	3	3*	5	5	4*	4	5	2*	2	1*	1		4	5	2		1	3	1		2
169	DIPROPYLENE GLYCOL, METHYL ETHER							3	4	2	5	3	5					5		5	2	3						5
170	~~%DECANE~~										2		0							5		5				1		
171	3,3,3-TRICHLOROPROPENE							0						4			5	1										
172	2-ETHYL-3-METHYLFUMARIC ACID												4			5	4					5						
173	ETHYL LACTATE															5												
174	DIACETYLBENEZENE															5												
175	ALDOL															5												
176	%1-(ETHENYLOXY) BUTANE															5												
177	6-PROPYL-BETA-RESORCYLIC ACID																5											
178	4-ISOPROPYL-O-PYROCATECHUIC ACID																5											
179	HEXAN-3-ONE							0				3	3	3				5		4	4							
180	2,5-HEXANEDIOL			2	3	3															1				5		2	

(Continued)

TABLE 11. (COntinued)

FINAL REPORT (PART I)

RELATIVE SIZE AND CONCENTRATE WHERE DETECTED

	COMMON NAME	*	V1C	V1X	T2B	T1C	T1X	T1Y	T4C	T4X	M2C	N2C	P2C	P2X	O2C	O2X	S2C	S2X	L2M	C3C	C1M	C1N	C2N	R1C	R2C	E1C	D2N	B2C	B3C
181	TETRAHYDRO-1,1-DIOXIDE THIOPHENE																												
182	N-TRIETHYLENE GLYCOL, MONOETHYL ETHER																							4	5				
183	METHYL MYRISTATE					1				1			2	5		4			2										1
184	METHYL STEARATE		1		1			5							3*										2*				
185	%*$STYRENE		1		2*		2	5																					
186	1,3-DIETHYL BENZENE			0	1			5	-1*				0*	1*	4		0*		2	1	1	2			1		1		
187	1,4-DIETHYL BENZENE	A		3	3			5*		3 *				2*	5	0									0				
188	1,2-DIETHYL BENZENE	A		4	3			5*		3 *				2*	5	1													
189	ETHYL PALMITATE	A		3	2			5*		2 *				2*	5	1													
190	METHYL-3,5-DIMETHYL BENZOATE	A		3	1			5*	-1	3 *				5*		5*		1							4				
191	2-METHOXY-3-METHYLCROTONIC ACID				3			5																					
192	%DIBROMOCHLOROMETHANE					3	3	5		4	3			2		3		4			3	2							2
193	2-CYCLOHEXENONE					3		5	0		5	5	3				1												
194	2,3,5,6-TETRACHLOROTEREPHTHALIC ACID					4		5			5	5	5						2			4	2	3					2
195	%$M-XYLENE						5	5		4																			
196	%3-CHLORO-2-METHYL PROPENE							5	1						2		2					3	3				1		2
197	%+$O-DICHLORO BENZENE							5																					
198	%*+$HEXACHLORO-1,3-BUTADIENE							5			3		1		1		2			1							0		
199	P-METHYLSULFONYL TOLUENE							5				1																	
200	1,1,3,3-TETRAMETHYL-2-INDANONE							5																					
201	2,3-DIMETHYL-2-BUTANOL							5																					
202	METHYL HEPTANOATE							5				4					2												
203	PHENYL ACETIC ACID, METHYL ESTER							5																					
204	DI-(2-BROMOETHYL)ETHER							5																					
205	1-ISOCYANO-4-METHYLBENZENE							5																					
206	SULFONYLBIS(4-CHLOROBENZENE)							5																					
207	2-ETHYL-4-METHYL-1-PENTANOL							5																					
208	3-METHYLCYCLOPENTANONE					3	5																						
209	%CAPROIC ACID					4	5							2		2		2	4*			1*							
210	%*+PHENOL		-1		1	5	4	2*	5	5	4	5	5	4	5	4	3*		4				4		5	3*	5	3*	5
211	2,3,3-TRICHLORO-2-PROPENOIC ACID			2		5	4	3	4	4	3	4			1	4			4	3	5	5	5					3	3
212	N-HYDROXYPHTHALAMIDE					5	4	3		4			5	4				4											3
213	1-ETHOXY-1-METHOXYETHANE					5	4			4																			
214	1-1-DIMETHOXYPROPANE					5																							
215	~~2,3-DIMETHYLMALEIC ACID~~ SEE NO. 32					5																							
216	ISOPROPYL BENZOATE					5																							
217	BENZOTHIAZOLE					5													3										
218	1,1-BIS(4-ETHYLPHENYL)ETHANE		1			3*		3	3*				4*				3*		3*		5*	5*	5*	3*			2*		
219	ADIPIC ACID, DIHEXYL ESTER	A		5						3*				4*		3*													
220	%+$BUTYL BENZYL PHTHALATE				3	4*	2*									3*								3	5				
221	4-ETHYLSTYRENE										5	4								5	4		2					5	
222	%STILBENE (CIS OR TRANS, SEE NO. 515)	A		5	1			3*		4*				5*	5	4*													
223	ISOPENTADECANOIC ACID	a		5										2*		0*													
224	%*+$PENTACHLOROPHENOL		0																						5		3		
225	2-HYDROXY DECANOIC ACID		0			1		2	2*			4		0	4		1*				4*	4*	5		1*	1*		1*	
				1																					5		3	4	

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TABLE 11. (Continued)

FINAL REPORT (PART I)

RELATIVE SIZE AND CONCENTRATE WHERE DETECTED

	COMMON NAME	*	V1C	V1X	T2B	T1C	T1X	T1Y	T4C	T4X	M2C	N2C	P2C	P2X	O2C	O2X	S2C	S2K	L2M	C3C	C1M	C1N	C2N	R1C	R2C	E1C	D2N	B2C	B3C
226	XMETA-CRESOL			1																								2	5
227	3,4-DICHLOROBENZOIC ACID			0				3*				4					2					5					3	2	
228	2-HEPTENYLBENZENE	A		5										3*		1*													
229	X2-METHYLNAPHTHALENE	A		5			2*		-1	2*	1	2	1	5*	1	3*	0			2	2	1		1	1				4
230	XBIPHENYL	A		5	1			3*	1	3*		3	0	5*	3	4	0	-1	1		4	2	2	1	3		2		1
231	2-METHYL BIPHENYL	A		5						4*		2		5*											0				
232	3,4'-DIMETHYL-1,1'-BIPHENYL	A		5																1									
233	XSTILBENE OXIDE	A		5						2*				5*		3*													
234	1,1-BIS(M-ETHYLPHENYL)ETHANE	A		5																									
235	ANTEISOPENTADECANOIC ACID				1			4																3	5		3		3
236	XCYCLOPROPYL METHYL KETONE				5							4			2														
237	2-METHYLCYCLOPENTANOL (GEOMETRY UNKNOWN)				5						5		4			1							4					3	
238	1-HEPTADECANOL				2												2				5						1		
239	X*$P-CHLOROPHENOL					2		3	3				4		2				1		5	4			1	2			
240	2,3-DIMETHYLBENZOIC ACID					4						4	5	2	5		3					5							
241	PHENOXY ACETIC ACID					4				5												5	5						
242	X1,4-DIOXANE					3*					5*	4*			2*	2*					2*		5*	3*					2*
243	X*2,4-DICHLOROPHENOXYACETIC ACID, (2,4-D)					1		3	3			4			4	3						5			1		2		
244	2-(2-HYDROXYPROPOXY)-1-PROPANOL (A DIPRO					4				1	4											5			2				
245	CYCLIC TETRAMETHYLENE ADIPATE					4			4										3		5								
246	1-CYCLOPENTYLETHANONE					4									2		3												5
247	METHYL N-AMYL KETONE						4		-1		4	4						1			4				2			5	
248	2-METHOXY-4-METHYL-2-PENTENOIC ACID						4	4		5	3			2	3	4		4			5	4							4
249	2,4,6-TRIMETHYLBENZOIC ACID							2	3		2		5		3		2		2			5							
250	ORTHO-TOLUIC ACID								3		4	4	5		3		4	3	4	3		5	5	3	4	2	1	2	
251	2-PHENYLPROPIONIC ACID								3	3													5		4		2		
252	XHYDROCINNAMIC ACID								4	3		4	5						3				5				2		
253	3,4-DIMETHYLBENZOIC ACID								4				5		4		3		2					5					
254	2,5-DIMETHYLBENZOIC ACID								3				2	1	3	3	3			2		4	5	2				4	
255	3-METHYL-2-HEPTANOL								2								2					5							3
256	XBENZYL ALCOHOL								3	4	5	5						1			2			4	5		3	3	4
257	BIS(2-ETHOXYETHYL)ETHER								3										5										4
258	X*O-CHLOROANILINE								0	1							2			2	5				1	1			
259	3,3-DIMETHYLBUTYRIC ACID									4	4	3	3	2			3		5				4						2
260	XSACCHARIN									3												5	5						2
261	2-ETHYLBUTYRIC ACID										2	3							4			5							2
262	CHRYSANTHEMIC ACID										4												5						
263	XPENTABARBITAL										5								3		5				4				
264	TRANS-9-HEXADECENOIC ACID										5						3				4	5							
265	2-PHENYLBUTYRIC ACID											4							4	3		5	5		3				
266	PHTHALIDE												5				3				4	5			2				2
267	2-HEXANOL												3	3	5				5										
268	TRI-N-PROPYLENE GLYCOL, METHYL ETHER												2						5										
269	2-(2-METHOXYPROPOXY)-1-PROPANOL (A DIPR													1								3	5						3
270	XN-UNDECYLIC ACID														2						3			5	4			3	

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TABLE 11. (Continued)

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RELATIVE SIZE AND CONCENTRATE WHERE DETECTED

	COMMON NAME	*	V1C	V1X	T2B	T1C	T1X	T1Y	T4C	T4X	M2C	N2C	P2C	P2X	O2C	D2X	S2C	S2X	L2M	C3C	C1M	C1N	C2N	R1C	R2C	E1C	D2M	B2C	B3C
271	7-OCTEN-2-ONE														2														5
272	~~%CHLOROFORM~~														~~3~~	~~3~~					~~5~~								
273	%METHYLPHENYL CARBINOL															1													5
274	DIOCTYL AZELATE																1											5	
275	3-METHOXY-1,2-BENZISOTHIAZOLE																	3		4	5								
276	2-METHYL-3-HEXENOIC ACID																		2				5						
277	5-PHENYL PENTANOIC ACID																		5										
278	TETRAHYDROFURAN-2,5-DICARBOXYLIC ACID																		5				3						
279	%ETHYL ACETATE																		5										
280	%METHYL ISOBUTYL KETONE																		5										
281	N-BUTYL ACETATE																		5										
282	4-ETHOXYBUTYL BUTANOATE																			5									
283	*TRICRESYL PHOSPHATE (ISOMER UNKNOWN)																			2					1			5	
284	$M-CHLOROPHENOL																				5								
285	4-(1,5-DIMETHYL-3-OXOHEXYL)CYCLOHEXANECA																				5				4*				
286	1,2-BENZISOTHIAZOL-3(2H)-ONE																				5								3
287	1,3-DIMETHYL BUTABARBITAL																				5								
288	1-PHENYL-1,2,3-PROPANETRIOL																				5								
289	N,N-DIMETHYLHEPTANAMIDE																				5								
290	%METHYL CHLOROFORM																					5							
291	2,2-DIMETHYL-1-BUTANOL																					5							
292	~~SUBERANE~~																					~~5~~							
293	2-TERT-BUTYLCYCLOHEXANOL																						5						
294	%ADIPIC ACID																						5						
295	2,2-DIMETHYLVALERIC ACID																						5						
296	ETHENYL CYCLOPENTANEACETATE																						5						3
297	(2,5-DIMETHYLBENZENE)BUTANOIC ACID																							4	4	1	3	5	
298	%ARACHIDONIC ACID																							3	5				
299	TRIPROPYLENE GLYCOL, METHYL ETHER																							5					3
300	%P-METHOXY-T-BUTYL PHENOL																							5					
301	3-BUTYL-6-METHYL-2,4-PYRIDINEDIOL																							5					
302	1-((2,6,6-TRIMETHYL-1-CYCLOHEXEN-1-YL)OX																								5				
303	ANTEISOHEPTADECANOIC ACID																								5				
304	TETRAETHYLENE GLYCOL MONOBUTYL ETHER																								5				
305	8,11-OCTADECADIENOIC ACID																								5				5
306	LIGNOCERIC ACID																								5				3
307	MYRISTYL ALCOHOL																										5		
308	3-METHOXY-2-BUTANOL																											5	
309	1,5-BIS(T-BUTYL)-3,3-DIMETHYL BICYCLO(3.																											5	
310	OCTADECATRIENOIC ACID																												5
311	ACENAPHTHYLENE																												5
312	PIPERIDINOL																												5
313	DIETHYL CARBINOL							2*		3*	5	4		3		4													
314	2,3-DIHYDRO-4-METHYLFURAN							3		2				5		2													
315	ETHYLBENZALDEHYDE	A	4	2			4*		4*				5*	1	4*		1*												

* SEE FOOTNOTE ON LAST PAGE

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TABLE 11. (Continued)

FINAL REPORT (PART I)

RELATIVE SIZE AND CONCENTRATE WHERE DETECTED

	COMMON NAME	V1*C	V1X	T2B	T1C	T1X	T1Y	T4C	T4X	M2C	N2C	P2C	P2X	D2C	O2X	S2C	S2X	L2M	C3C	C1M	C1N	C2N	R1C	R2C	E1C	D2N	B2C	B3C
316	2',3'-DIMETHYLACETOPHENONE	A											4*		5*		1*											
317	3-ETHYLSTYRENE	A	4	2					4*			1	4*	5	4*													
318	ETHYL MYRISTATE	A	4				4*		2*				4*	5	3*		1*							2				
319	DECAHYDRO-2,3-DIMETHYLNAPHTHALENE			2			3							5														
320	%'(2,4,5-TRICHLOROPHENOXY)ACETIC ACID				1		3	0			4			5										1				
321	3,4-DIMETHYL-2,5-FURANDIONE								3		4			5														2
322	1,2,3-TRIMETHYL-4-PROPENYLNAPHTHALENE (T	a							4*	1	2				5		3						2	1				
323	DIETHYLENE GLYCOL, MONOMETHYL ETHER (C												3	5	4	4	0	3	1	4				1				3
324	3-ETHYL-4-METHYL-1H-PYRROLE-2,5-DIONE													5														
325	2,3-DIMETHYLMALEIMIDE													5														
326	5,6-DIMETHYL-1-INDANONE													5														
327	4A,5,6,7,8,8A-HEXAHYDRO-4A,8A-DIMETHYL-2													5	5													
328	%O-CRESOL														5													4
329	4,4-DIMETHYLDIHYDROFURANONE									5																		4
330	3-METHYLPENTAN-3-OL	0				4	3				3*	5				2*	2	3*			2*							
331	2,5-HEXANEDIONE				3	3		1		3		5	2	4		4	3	3		3	4	2	2		4	0		1
332	VERATRIC ACID		1					2					5			2	3											
333	%1-METHYLNAPHTHALENE	A	4				1*		1*		2	1	5*	0	3*	-1			1	2	1		1	1				0
334	(1-NITROPROPYL)BENZENE		4										5*															
335	2,5-DIMETHYLBENZALDEHYDE	A	4	1			3*						5*	3	4*		0											
336	3-METHYLBIPHENYL	A	1										5*															
337	ETHYL LAURATE	A					4		2				5*	2	4*		1*											
338	2-ETHYL INDAN	A											5*															
339	2,2,5,7-TETRAMETHYL TETRALIN	A											5															
340	BENZYL METHYL KETONE												5		4	1												
341	3,5-DIMETHYLBENZOIC ACID		1	1				3		3		5	3*		4*	3	2*	2	3	3	3	4	2	3		2		
342	DIISOBUTYL KETONE		2									5									1							
343	2,2,6-TRIMETHYL-1,4-CYCLOHEXANEDIONE					3		3	3	5		5	4	4	4	4	2											3
344	5-METHYL-2-HEPTANOL						4					5																
345	ISO-HEXANOIC ACID									3	3	5	3	2	2						4		2					
346	HEXAHYDROBENZOIC ACID									4		5	3				1									2		3
347	%2-PHENYLISOPROPANOL									4	5	5	4										3	3				
348	1-(2-METHOXY-1-METHYLETHOXY)-2-PROPANOL										3	5												1				4
349	4-METHYLHEXANOIC ACID											5		1		2												
350	3-METHYLPENTANAL											5												3				
351	~~ISOBUTYLCYCLOHEXANE~~											5																
352	2,2-DIMETHYL-1-PENTANOL											5				-1												
353	2-(2-METHOXY-1-METHYLETHOXY)-2-PROPANOL											5																4
354	1-(ETHENYLOXY)HEXANE											5		3		4												
355	FENCHYL ALCOHOL											5																
356	%MENTHOL											5																
357	1-(TRIMETHYLOXIRANYL)ETHANONE											5																
358	%ENDO-BORNEOL											5												3				
359	1,2 3,5-BIS-O-(1-METHYLETHYLIDENE)-ALPHA											5																
360	4-NONANOL											5																

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TABLE 11, (Continued)

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RELATIVE SIZE AND CONCENTRATE WHERE DETECTED

	COMMON NAME	V1C	V1X	T2B	T1C	T1X	T1Y	T4C	T4X	M2C	N2C	P2C	P2X	O2C	O2X	S2C	S2X	L2M	C3C	C1M	C1N	C2N	R1C	R2C	E1C	D2N	B2C	B3C
361	OCTAHYDRO-4A,5-DIMETHYL-3-(1-METHYLETHYL											5																
362	NONADECANOL											5																
363	ANISIC ACID		0				4	4	4		5	4	3*		3*	2									1	2	2	
364	5,6,7,7A-TETRAHYDRO-4,4,7A-TRIMETHYL-2(4				3			4			5	4	4			3							3					
365	1,3-DICHLORO-2-METHYLBUTANE (A DICHLO							2		5	5	4				0	2											
366	DIPROPYLENE GLYCOL, METHYL ETHER							2	4	4	5	3	4					5		3		2	3					4
367	5,5-DIMETHYL-2-FURANONE							3		5	5					3												3
368	XTCA(TRICHLOROACETIC ACID)										5					4												
369	DICHLOROPHENOXYACETIC ACID (ISOMER UNKNO										5																	
370	PIVALIC ACID										5	3				4												
371	3-CHLOROCYCLOPENTENE										5																	
372	6-(ACETYLOXY)-2-HEXANONE										5						-1											
373	6,7-DODECANEDIONE										5					4												
374	DIETHYL PENTYL PHOSPHATE										5																	
375	7-TRIDECANONE										5																	
376	XLAURYL ALCOHOL										5	3				3	2							2		3		
377	N,N,4-TRIMETHYLBENZENESULFONAMIDE										5																	
378	ISOPROPYL HYDROPEROXIDE										5																	
379	3,4-EPOXY-2-HEXANONE	2								5*						2*	2*				4*				3*			
380	X+$DIHEXYL PHTHALATE	0								5																		
381	LEVULINIC ACID				2	4	3	4		5	3	3	3	3	3	3	4			3	3							2
382	1-HEPTEN-4-OL					3				5						3												
383	2-METHYL-1-PENTEN-3-OL					4				5						4		1			2							
384	N,N-DIETHYL FORMAMIDE							3	3	5				1		3	1						3					
385	2-METHYL-2-HEPTANOL								1	5						1												
386	3,5-DIMETHOXYPHENOL									5																		
387	XAMOBARBITAL									5								4		4								3
388	PETROSELINIC ACID									5																		
389	XCYCLOHEXYL BROMIDE									5		2				0	2											
390	5-METHYL-3-HEXANOL									5							1											
391	2-METHYL-2-BUTEN-1-OL									5		4				2												
392	5-ETHYL-2-HEPTANOL									5																		
393	3-METHOXY-1,3,4-HEXATRIENE									5																		
394	2-METHYL-2-ISOBUTYLOXIRANE									5																		
395	1-METHYLHEXYLHYDROPEROXIDE									5																		
396	2-BUTYL-3-METHYLOXIRANE									5											3							
397	2-METHOXY-4-METHYL-2-PENTENOIC ACID, MET									5	4																	
398	2,3,4-TRIMETHYL-3-PENTANOL									5																		
399	1-ISOCYANONAPHTHALENE									5																		
400	N-TERT-BUTYL-3-METHYLBENZAMIDE									5																		
401	4,5-DIETHYL-2,3-DIHYDRO-2,3-DIMETHYLFURA									5																		
402	4,7-DIMETHYL-1,3-ISOBENZOFURANDIONE									5																		
403	2,5-DIMETHYL-2-HEXANOL									5																		
404	PROPYLOXIRANE									5																		
405	XCYCLOHEXYL ACETATE									5	1	1				1												

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TABLE 11. (Continued)

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RELATIVE SIZE AND CONCENTRATE WHERE DETECTED

	COMMON NAME	*	V1C	V1X	T2B	T1C	T1X	T1Y	T4C	T4X	N2C	N2G	P2C	P2X	O2C	O2X	S2C	S2X	L2M	C3C	C1M	C1N	C2N	R1C	R2C	E1C	D2N	B2C	B3C
406	X(ETHOXYMETHYL)OXIRANE										5																		
407	4-HEPTANONE						5*								3*	1*	1*		3*	3*		2*							
408	4,6-DIMETHYL OCTANOIC ACID								5																			2	
409	O-CRESYL ACETATE								4	5																		3	
410	3-HYDROXYNONANOIC ACID								5																			3	
411	X2,4-DIMETHOXYBENZOIC ACID	A								5								2											
412	P-ETHYLBENZOIC ACID									5*																			
413	4-HYDROXY-4-METHYLCYCLOHEXANONE					2																							5
414	X*P-CRESOL		0	0					0*	0*																		4*	4*
415	1,1-DIPHENYLETHANE	A		4						4*		2		1*	0	0*		2*											
416	2-BUTYL THF								-1		3						4	2				4						2	
417	METHYL AMYL CARBINOL			1									4*				4*						2*					4*	3*
418	%ETHYL CARBONATE							3					4				4												2
419	5-METHYL HEXANOIC ACID							2				3	4		3		4			2				2			4		2
420	4,5-DIMETHYL-2-HEPTEN-3-OL										2						4												
421	5-METHYL-2-HEPTANONE										4						4											2	1
422	1,3,3,7-TETRAMETHYL-2-OXOBICYCLO(2.2.1)H												4				4												
423	BUTYL ISOBUTYRATE												3				4												
424	2-ETHYLCYCLOHEXANONE														4		4												
425	DIETHYLENE GLYCOL, METHYL ETHYL DIETHER																4												
426	2-METHYLHEPTANOIC ACID																4												
427	1,6-HEXANEDIOL																4					3							
428	2,3-DIHYDRO-4-(1-METHYLETHYL)FURAN																4												
429	CYCLOHEXANEHEXANOL																4												
430	~~2,5-DIMETHYLHEXANE~~																4												
431	2,2,5,5-TETRAMETHYL THF																4					3							
432	X4(1H)-PYRIMIDINONE																4												
433	3,5-NONADIEN-7-YL-2-OL																4												
434	4,4,5,5-TETRAMETHYL-1,3-DIOXOLAN-2-ONE																4												
435	2-(1-METHYLETHYLIDENE)CYCLOHEXANONE																4												
436	OXACYCLOTETRADECAN-2-ONE																4												
437	1,1-DICHLORO-2-HEXANONE																4												
438	4,4-DICHLORO-3-HEXANONE																4												
439	DIHYDRO-5-METHYL-2(3H)-FURANONE																4												3
440	C3-DIHYDROXYBENZOIC ACID																	4											
441	4-BUTOXYBUTYRIC ACID																	4						3					4
442	X$1,2-DICHLOROETHANE					3		2								4							4						
443	PENTAETHYLBENZENE			4																									
444	XDMF (DIMETHYL FORMAMIDE)										2		2				1				4	2	3				2		
445	N-ACETYLCYCLOHEXYLAMINE																								4				
446	O-ETHYLBENZOIC ACID	A		3				4*		4*																			
447	X+$DICHLOROETHYL ETHER			-1				4						1*		0*													
448	XETHYL BENZOATE	A		4	1			4*						2*	2														
449	ETHYL PENTADECANOATE	A		2				4*		2*				3*		2*													
450	ETHYL STEARATE	A		2	1			4*		2*				3*		3*													

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TABLE 11. (Continued)

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RELATIVE SIZE AND CONCENTRATE WHERE DETECTED

	COMMON NAME	*	V1C	V1X	T2B	T1C	T1K	T1Y	T4C	T4X	M2C	N2C	P2C	P2X	O2C	D2X	S2C	S2X	L2M	C3C	C1M	C1N	C2N	R1C	R2C	E1C	D2N	B2C	B3C
451	%*+$P-DICHLOROBENZENE																												
452	METHYL LAURATE				1	1		4	8		2	4	8				-1	2		1		2							
453	METHYL-2,4-DIMETHYL BENZOATE	a			3			4*																	1				
454	2,3-DICHLOROANILINE	a			2			4*																	2				
455	%$DIMETHYL PHTHALATE					3		4		2			2				1												
456	%BENZYL CYANIDE					4		4																					
457	3-HEPTANOL					2		4			2	4	4				1			4		1		4	4	2		4	4
458	1-CHLORO-2-METHYL-2-BUTENE						3	4																4	3			1	
459	NEOPENTYL CHLORIDE							4										-1						3				4	2
460	1-BROMO-4-ETHYLBENZENE							4			2																		
461	2,4,5-TRICHLOROANILINE							4																					
462	*PENTACHLOROANILINE							4									1							2					
463	1,2,2,3-TETEACHLOROPROPANE							4																					
464	%*+$1,2,4-TRICHLOROBENZENE							4	2																				
465	2,4-DICHLORO-1-NITROBENZENE							4			2		8				-1	2				1			1				
466	+%LINDANE (BETA ISOMER)							4									8												
467	%*PENTACHLORONITROBENZENE							4				3																	
468	DIMETHYL AZELATE							4																					
469	4-TERT-BUTYL-2-METHYLPHENOL							4																					
470	4-METHYLPHENYLSULFONYL ACETIC ACID, METH							4	0							4	2												
471	4-METHYL-1-PHTHALAZINONE							4																					
472	2-METHYL-2-PENTANOL							4																					
473	%CAMPHOR							4			4	4			1		2												
474	PENTYLENETETRAZOLE							4									2												
475	SUCCINIC ACID, DIMETHYL ESTER							4							3														
476	%DIETHYL SUCCINATE							4																					
477	2,2-DIMETHYLGLUTARIC ACID							4																					
478	1-(METHYLPHENYL)ETHANONE							4																					
479	METHYLSULFONYL BENZENE	A						4*		2*						2*					4		4						
480	ALLYL-1,3-DIOXANE							4																					
481	METHYL CAPROATE							4																					
482	METHYLCAPRYLATE							4																					
483	METHYL PELARGONATE							4															2						
484	ETHYLNONENOATE							4																					
485	METHYL CAPRATE							4																					
486	BENZONITRILE							4																					
487	PHENYLPROPIONIC ACID,METHYL ESTER							4					2								2								
488	2,4,5-TRICHLOROPHENOXY ACETIC ACID, METH							4																					
489	2,2-DIMETHYL-3-PENTANOL							4																					
490	(1-ETHOXYETHYL)BENZENE							4																					
491	1,2-DIMETHYL-4-NITROBENZENE	a						4*								4*		-1					3						3
492	METHYL HEPTADECANOATE (METHYL MARGARAT							4																					
493	2-HEXENOIC ACID							4																					
494	%DALAPON					4	4	3						2															4
495	HENEICOSANIC ACID						4	3		3							3	3											
							4																		3				3

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TABLE 11. (Continued)

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RELATIVE SIZE AND CONCENTRATE WHERE DETECTED

	COMMON NAME	*	V1C	V1X	T2B	T1C	T1X	T1Y	T4C	T4X	M2C	N2C	P2C	P2X	O2C	O2X	S2C	S2X	L2M	C3C	C1M	C1N	C2N	R1C	R2C	E1C	D2N	B2C	B3C
496	HEPTYL ALCOHOL						4		2														2						
497	6-UNDECANOL					4	3							3			-1												
498	P-ISOPROPYL BENZOIC ACID					4			3				2				3			2							2	2	
499	4,4-DICHLOROBUTENOIC ACID					4				3			4	2				3											2
500	%ANTHRANILIC ACID					4																							4
501	2-METHYL-4-(2,5-XYLYL)BUTANOIC ACID					4																							
502	2-PHENOXYETHANOL					4																							
503	(2-ETHOXY-1-METHOXYETHOXY)-ETHENE					4																							
504	N,N'-DIMETHYLUREA					4																							
505	2,6-DI-T-BUTYL-P-BENZOQUINONE		-1	1		2			2*			3*	2*				1*		2*	2*	4	2*		3*			1*	2*	2*
506	DIPHENYLMETHANE	A		4						3*				3*		3*													
507	%CAFFEINE								4	3		4	4						4			3		3					
508	1,2-DIHYDRONAPHTHALENE	A		4										3*		1*													
509	TETRAETHYLBENZENE	A		4						3*				4*		3*													
510	1-ETHYLNAPHTHALENE	A		4										4*		2*													
511	1-METHYL-7-ISOPROPYL NAPHTHALENE	A		4																		2							
512	%3-METHYLPHENANTHRENE	a		4										2*											2				
513	1-PHENYL TETRALIN	A		4						1*				3*		2*													
514	1,1-BIS(O-ETHYLPHENYL)ETHANE	A		4																									
515	%STILBENE(TRANS OR CIS, SEE NO. 222)	A		4										4*		2*													
516	2-PHENYL TETRALIN	A		4						1*				3*		2*													
517	3-ETHYLACETOPHENONE	A		4						3*						4*													
518	2-(ETHYLPHENYL)PROPYL METHYL ETHER			4																									
519	2-METHOXY-1-PROPANOL		0																					4*				2*	
520	ISOMYRISTIC ACID		0																						4*				
521	9-KETOCAPRIC ACID		-1											2*	4									3*	4	2*	4	3*	
522	ISOPALMITIC ACID		-1																						4				
523	%P-CHLOROBENZOIC ACID			3				3				4	3							4		3				2	4		
524	%CETYL ALCOHOL				3				1*				1*			2*	2*										4*		
525	%ETHYLENE TETRACHLORIDE				4				3																1				
526	2-METHOXY-3-METHYL-2-PENTENOIC ACID					3	3	3		3				2		3		3			4	3							4
527	4-OXO-NONANOIC ACID					3																			4		3		
528	3-METHYL-2-CYCLOHEXEN-1-ONE					2			3				1	4		2	2	2											4
529	BUTYLBENZYLPHTHALATE					3																		4					
530	2-METHYL-2-PROPYLHEXANOIC ACID							2			4										4								
531	M-CHLOROBENZOIC ACID							3	3													3		3	4		1		
532	%CHLOROBENZENE							3	0			1					-1					4							
533	BETA,BETA-DIMETHYLPHENYLACETIC ACID								3																4				
534	3-PHENYL PENTANOIC ACID								3										4			3					2		
535	%*+$2,4-DICHLOROPHENOL								0			3	4								4				1			1	
536	4-HYDROXY-4-METHYL-2-PENTANONE								2																				4
537	% PYRIDINE								1	4															4				
538	2,2-DIMETHYL BUTYRIC ACID									2		3					2		3		2	4				3			2
539	ACETOACETIC ACID									2						2							4						
540	2-(HYDROXYMETHYL)BENZOIC ACID									4								0					4				2		

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(Continued)

TABLE 11. (Continued)

FINAL REPORT (PART I)

RELATIVE SIZE AND CONCENTRATE WHERE DETECTED

	COMMON NAME	V1C	V1X	T2B	T1C	T1X	T1Y	T4C	T4X	M2C	N2C	P2C	P2X	O2C	O2X	S2C	S2X	L2N	C3C	C1M	C1N	C2N	R1C	R2C	E1C	D2N	B2C	B3C
541	TERPIN								1				3															4
542	3-METHYL VALERIC ACID				4	2				4		3	4	1	3			3		4								2
543	3-METHOXYBENZOIC ACID										4	2																4
544	3-HYDROXYTETRADECANOIC ACID										4			4													4	
545	2,6-DICHLOROBENZOIC ACID										4																4	
546	UNDECANEDIOIC ACID										4		3		3								4	4		4	3	
547	5-EPIDEOXYPODOCARPIC ACID										2			3		3				4								
548	DIACETONE ALCOHOL										4	4				2		2*			3*		4*					2*
549	3-OCTANONE										3	1	1			0			4									
550	3-OCTENOIC ACID											4						4										
551	O-ANISIC ACID											4	2	4	3													4
552	DICYCLOHEXYLADIPATE											3						1										4
553	5-METHYL-2-HEXANOL												3												4			
554	PIPERIDINONE													4									4					2
555	TRIDECYLIC ACID													2		2							3	4		2		
556	HEXAHYDRO-4-METHYL-2H-AZEPIN-2-ONE													2							4							
557	%P-TERT-BUTYL PHENOL															2				4								
558	VACCENIC ACID															3								4				
559	6-METHYL-3(2H)-BENZOFURANONE															2					4	3						
560	1,3-DIMETHOXY-2-PROPANOL															3				4								
561	DIMETHYLSULFONE															2				4	2	2	3	2		1		3
562	P-(1,1,3,3-TETRAMETHYLBUTYL)PHENOL															-1	0	1		4	4							
563	3-METHOXY-2-METHYL-2-PENTENOIC ACID																3				4							
564	3,3 DIMETHYLGLUTARIC ACID																	4										
565	%$BUTYL(BUTOXY CARBONYL) METHYL PHTHALATE																	4										
566	$DIMETHYL TEREPHTHALATE																	4	2									
567	$TERT-BUTYL METHYL PHTHALATE																		4									
568	%2-HYDROXYBIPHENYL																		4									
569	CIS-2,5-DIMETHYLTETRAHYDROFURAN																			4								
570	N-METHYLETHOSUXIMIDE																			4								
571	4-TERT-BUTYL-O-PHENYLENE CYCLIC CARBONAT																			4								
572	BUTABARBITAL																			4								
573	2,6-BIS(1,1-DIMETHYLETHYL)-4-ETHYLPHENOL																			4								
574	ANISOLE-2-ACETIC ACID																			4								
575	BETA,3,4-TRIMETHYLBENZENEPROPANOIC ACID																			4								
576	4-(1,5-DIMETHYL-3-OXOHEXYL)-1-CYCLOHEXEN																			4				2		4		
577	2-(PHENYLMETHYL)BENZOIC ACID																			4								
578	BENZOFURANONE																			4								
579	1,3-PROPYLENE GLYCOL, BUTYL METHYL DIETH																			4								
580	ALPHA,ALPHA-DICHLOROPHENYLACETIC ACID																				4			2				
581	%P-TOLUENESULFONAMIDE																				4							
582	1-(2-BUTOXY-1-METHYLETHOXY)-2-PROPANOL (																				4							
583	6-METHYL-TETRAHYDRO-2-PYRANONE																				4							
584	~~3,3-DIETHYLPENTANE~~																				~~4~~							
585	1-METHOXY-2-HEXENE																				4							

(Continued)

TABLE 11. (Continued)

FINAL REPORT (PART I)

RELATIVE SIZE AND CONCENTRATE WHERE DETECTED

	COMMON NAME	*	V1C	V1X	T2B	T1C	T1X	T1Y	T4C	T4X	M2C	N2C	P2C	P2X	O2C	O2X	S2C	S2X	L2M	C3C	C1M	C1W	C2W	R1C	R2C	E1C	D2N	B2C	B3C
586	DI-N-HEXYL ETHER																					4							
587	1-METHOXY-2-BUTANOL																						4						
588	2,3-DIMETHYL-3-PENTANOL																						4						
589	2-METHYLGLUTARIC ACID																						4						
590	2-ACETYL-4-METHYL-4-PENTENOIC ACID																						4						
591	2,6-DIMETHYLPHENOXY CARBONIC ACID																						4						
592	X6-HYDROXYCAPROIC ACID LACTONE																						4						
593	2,3-DIMETHYLTETRAHYDRO-2-FURANOL																							3				4	
594	XTRIMETHYL NITROSO UREA																							4					
595	3,4-DIHYDROXY-6-METHOXY-1-NAPHTHALENONE																							4					
596	XMESITYL OXIDE (3-ISOHEXEN-2-ONE)																							4					
597	1-ETHOXY DECALIN																								4				
598	NONADECANOIC ACID																								4				
599	BEHENIC ACID																								4				2
600	1,3,6-TRIOXOCANE																								4				
601	2-ETHYL-1,3-HEXANEDIOL																								4				
602	2-ETHYL-5-METHYLDIOXANE																								4				
603	4-HEXEN-2-ONE																									4			
604	3-HYDROXY-1,2-BENZISOTHIAZOLE																											4	
605	O-PROPIONYL BENZOIC ACID																											4	
606	2-METHYL-4-DIBROMOMETHYL BENZOIC ACID																											4	
607	2-AMINO-5-CHLOROBENZOIC ACID																												4
608	2,3-BUTANEDIOL																												4
609	EXO-BORNEOL																												4
610	2,2,3-TRIMETHYL-3-CYCLOPENTENE-1-ACETALD																												4
611	DICYCLOHEXYL SEBACATE																												4
612	2,6,6-TRIMETHYL-1-CYCLOHEXENE-1-CARBOXAL														4														
613	TRIETHYLENE GLYCOL METHYL ETHER													4															
614	1,3,5-TRIETHYLBENZENE	a		3						3*				4*	3	4*													
615	2,6-DIMETHYL DECALIN				1										4														
616	XBUTROLACTONE				3										4														
617	1,1,3-TRICHLORO-1-PROPENE					2			1		4	4	4		4		1	2				1							
618	SEBACIC ACID	a								3				3		4											3		
619	2,6-DIMETHYL ACETOPHENONE									2*						4*													
620	3-OCTEN-2-ONE												3		4														
621	2-METHOXY-3,5,5-TRIMETHYL-2-CYCLOHEXENE-														4	1		2											2
622	XSUCCINIC ACID															4													
623	2-ETHOXYNAPHTHALENE															4													
624	XN-DECYL ALCOHOL												4			2	2												
625	1,2,4-TRIETHYLBENZENE	A		3						3*				4*	2	3*													
626	TETRALIN	A		3	1			2*		2*		2	0	4*	2	3*	-1												
627	DIVINYLBENZENE	A		2						2*				4*	2														
628	P-ETHYLBENZALDEHYDE	A		2						4*				4*	3			-1*											
629	2*-METHYLACETOPHENONE	A		1								3		4*		2*													
630	1-METHYL TETRALIN	A		2						2*			0	4*			-1				1								

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TABLE 11. (Continued)

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RELATIVE SIZE AND CONCENTRATE WHERE DETECTED

	COMMON NAME	*	V1C	V1X	T2B	T1C	T1X	T1Y	T4C	T4X	M2C	N2C	P2C	P2X	O2C	O2X	S2C	S2X	L2M	C3C	C1M	C1N	C2N	R1C	R2C	E1C	O2N	B2C	B3C
631	1,1-DIMETHYL INDAN-4-CARBOXYLIC ACID, ET	A		1										4*		3*													
632	2-ACETYLOXYACETOPHENONE	a			2									4*															
633	2',4'-DIMETHYLACETOPHENONE	A						3*			4			4*		2*		8											
634	X2-ETHYL NAPHTHALENE	A								2*				4*		3*				1									
635	2-METHYL INDAN	A										2		4*	2														
636	2,2-DIMETHYL-3,5-DECADIYNE													4															
637	5-METHYL INDAN	A												4*			-1					1							
638	2,5-CYCLOHEXADIENYLBENZENE													4															
639	ALPHA-METHYLSTILBENE	a												4*															
640	2,3,4,5,6-PENTAFLUORO-N-(2-PHENYLETHYL)B													4															
641	4,4'-DIETHYLBIBENZYL	a												4*															
642	DIPROPYLENE GLYCOL METHYL ETHER (1-(2-													4					3										
643	3-PROPYLCYCLOPENTENE													4															
644	2-HENDECANOL													4		2													
645	1-UNDECANOL													4			2												
646	HEXYL BENZOATE													4															
647	PENTYL BENZOATE													4											3				
648	4-METHYLPHTHALIC ACID						2					4	4					1							2				
649	X2-NAPHTHOIC ACID								2			3	4				2												3
650	1,2,3,3-TETRACHLORO-1-PROPENE								-1		4		4				2												
651	1-METHYL-4-(1-METHYLETHYL)-7-OXABICYCLO(								2			4	4																
652	2-METHYL VALERIC ACID										2	2	4	2	1	1			2				3						
653	1-(4,5-DIETHYL-2-METHYL-1-CYCLOPENTEN-1-										4		4																
654	FENCHONE											4	4						3										
655	1-PHENYLBUTYRIC ACID												4							2									
656	2-HYDROXYTETRADECANOIC ACID												4																
657	3-METHYLPHTHALIC ACID												4																
658	4-METHYL-3-PENTENAL												4																
659	XCINEOLE												4																3
660	3-ETHOXY-3-METHYL-2-BUTANONE												4																
661	ISOPROPENYLBENZENE												4																
662	6-METHOXY-2-HEXANONE												4													2			
663	2,4-HEPTANEDIONE												4																
664	2-CYCLOOCTYL-2-PROPANOL												4																
665	METHYL 2,2,3-TRIMETHYLCYCLOPENTYL KETONE												4																
666	THIOHEXANOIC ACID, S-BUTYL ESTER												4																
667	3-ETHOXY-3-METHYL-1-BUTYNE												4		3		3												
668	5-(PENTYLOXY)-2-PENTENE												4		2														
669	2-ETHYL-3-METHYLOXETANE												4																
670	2-METHYL-2-PROPYL-1,3-DIOXOLANE												4																
671	2-ETHYL-1,3,2-DIOXABOROLANE												4																
672	BORNYL 2,5-DIKETONE												4																
673	7,7-DIMETHYL-11-DODECEN-2-ONE												4																
674	METHYL 9-OXODECANOATE												4																
675	CYCLOOCTANEPROPANOL												4																

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TABLE 11. (Continued)

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RELATIVE SIZE AND CONCENTRATE WHERE DETECTED

	COMMON NAME	V1C	V1X	T2B	T1G	T1X	T1Y	T4C	T4X	M2C	N2C	P2C	P2X	D2G	D2X	S2G	S2X	L2M	C3C	C1M	C1N	C2N	R1C	R2C	E1C	D2N	B2C	B3C
676	CYCLOHEXYL METHYL KETONE											4			1													
677	P-ISOPROPYLBENZALDEHYDE; CUMINALDEHYDE											4		3		8												
678	2,3 5,6-DI-O-ISOPROPYLIDENE-ALPHA-D-TALO											4																
679	1-TERT-BUTYL-4-ETHOXYBENZENE											4																
680	5-METHYL-1(3H)-ISOBENZOFURANONE											4				3												
681	9-OCTADECENAL											4																
682	4-METHYL-3-HEPTEN-2-ONE											4				2												
683	6-METHOXY-2-METHYL-3-HEXANONE											4																
684	2,6-DIMETHYL-3-HEPTANOL											4																
685	2-(2-METHOXY-1-METHYLETHOXY)-1-PROPANOL											4						2										1
686	AMYL BUTYL PHTHALATE											4																
687	2-ETHYL-2-ISOBUTYL-1,3-DIOXOLANE											4																
688	P-(1-HYDROXY-1-METHYLETHYL)ACETOPHENONE	0									4					2							3*					
689	2,2,6-TRIMETHYLCYCLOHEXANONE				2		4		2	4	4	3	3	2	2	2	8											
690	2,3-DIMETHYLBUTYRIC ACID						2		4	3	4	2	3	2	2	3	2											2
691	DICHLOROISOPROPYL ETHER						1				4																	
692	PENTACHLOROCYCLOPROPANE							2			4																	
693	2,3-OCTANEDIONE							3	3		4				2		-1											
694	~~1-ETHYL-2,3-DIMETHYLCYCLOHEXANE~~							4			4																	
695	BUTYLBENZOATE									3	4	1											3	3			2	
696	XCHLORODIBROMOMETHANE										4							3										
697	TRICHLOROPHENOXYACETIC ACID (ISOMER UNKN										4																	
698	3-BROMO-1,1-DICHLOROPROPANE										4																	
699	XTERT-PENTYL ALCOHOL										4																	
700	5-METHYLHEXANOL										4																	
701	CIS-3,4,4-TRIMETHYL-5-OXO-2-HEXENOIC ACI										4				3													
702	ETHYLENE GLYCOL, MONOMETHYL ETHER										4															2	3	
703	4-ISOPROPYLCYCLOHEXANOL										4																	
704	4-METHYL-3-HEPTANOL										4																	
705	SEC-BUTYLISOPROPYL ETHER										4									3								
706	X2-PROPENYL HEXANOATE										4																	
707	CYCLOPENTANONE										4																	
708	VINYL BUTYRATE										4																	
709	TETRAHYDRO-5-METHYL-2-FURANMETHANOL										4					2												
710	OCTAHYDRO-2,2,4,4,7,7-HEXAMETHYL-1H-INDE										4																	
711	OCTYL ACRYLATE										4					3												
712	XN-METHYL-2-PYROLIDONE					1		4	4									1										3
713	4-KETOISOHEPTANOIC ACID		1		3	3		3	4*	4	3		3*		3*	2	3*				3							2
714	3-METHYL-4-PENTEN-2-ONE				3					4							2											
715	CIS-1,3-DICHLOROCYCLOHEXANE									4																		
716	3,4-DIHYDRO-6-METHYL-2H-PYRAN									4																		
717	5-METHOXY-2-METHYL-2-PENTANOL									4		3																
718	2-VINYLCROTONALDEHYDE									4				2														
719	(1-METHYLBUTYL)OXIRANE									4																		
720	2-HYDROXYCYCLOHEXANONE									4																		

(Continued)

TABLE 11. (Continued)

FINAL REPORT (PART I)

RELATIVE SIZE AND CONCENTRATE WHERE DETECTED

	COMMON NAME	V1C	V1X	T2B	T1C	T1X	T1Y	T4C	T4X	M2C	M2C	P2C	P2X	D2C	D2X	S2C	S2X	L2M	C3C	C1M	G1M	C2M	R1C	R2C	E1C	D2M	B2C	B3C
721	5-METHYL-1-HEXANOL									4															3			
722	2-T-BUTYL-2-METHYL-1,3-DIOXOLANE									4																		
723	3-CHLORO-2-CYCLOPENTEN-1-ONE									4				2														
724	4,6,6-TRIMETHYLTETRAHYDRO-2-PYRANONE									4												3						
725	3,7-OCTADIEN-2-ONE									4																		
726	2-HEPTENOL									4																		3
727	2-BUTOXYPENTANE									4																		
728	ALPHA-ACETYLBUTYROLACTONE (GAMMA LACTONE									4																		
729	2-OCTEN-1-OL									4																		
730	CHLOROACETONITRILE									4																		
731	~~[illegible]~~ SEE NO. 541				4	2																						[illegible]
732	XCINNAMALDEHYDE		2						2*												4							
733	2-METHYLENEBUTYRIC ACID						1		4				2	2	3		2											2
734	XETHYLENE GLYCOL MONOETHYL ETHER) (OXITOL							4							1												3	
735	3,6-DIMETHYLOCTANOIC ACID (AN ISODECANOI							4												3							2	
736	3-METHYL-4-PHENYLBUTYRIC ACID							4										3										
737	OCTAHYDRO-1,4A-DIMETHYL-1-PHENANTHRENE C							4																			2	
738	1,3-DIMETHYL-2-(2-ISOPROPYLPHENYL)ETHYLC							4																				
739	X7-OXABICYCLO(4.1.0)HEPTANE							4		3																		
740	X1,2-DIHYDRO-3,6-PYRIDAZINEDIONE								4														3					
741	3-HYDROXYOCTANOIC ACID								4																			
742	3,4-DIHYDROXYBENZALDEHYDE								4																			
743	2,3-DICHLOROACRYLIC ACID								4																			
744	5-OXO-HEXANOIC ACID								4						2													
745	~~ACETIC ACID~~								4																			
746	X*ANILINE								4																			
747	X2,2,2-TRICHLOROETHANOL															3				3								2
748	XSP-XYLENE			3			3*							2		1	2	2*								1*		
749	4-ACETYLMORPHOLINE				3																			1				1
750	2-METHYLPHENYLPROPANOIC ACID		-1													3												
751	XTERT-BUTANOL		2													3												
752	3-METHYL-2-CYCLOPENTEN-1-ONE							3	2		3				2	3												
753	2,4-DIMETHYL-4-HEPTANOL									2						3												
754	2-METHYLCAPROIC ACID											1				3												
755	2,3,4,5,5-PENTACHLORO-2,4-PENTADIENOIC A											2				3	2											
756	2-METHYL-2-HEPTEN-4-ONE														1	3												
757	X2-ACETYLFURAN														1	3	1				3	3						
758	4-AMINO-3,5-DICHLOROBENZOIC ACID															3												
759	4-ETHYLHEXANOIC ACID															3												
760	XAMIBEN															3												
761	ETHYL ISOBUTYL KETONE															3												
762	XMETHYLAL															3								2				
763	3-METHYL-2-HEXANOL															3					1							
764	1-METHYL-4-METHYLENESUBERANE															3												
765	2,4-DIMETHYL-2-PENTENE															3												

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TABLE 11. (Continued)

FINAL REPORT (PART I)

RELATIVE SIZE AND CONCENTRATE WHERE DETECTED

	COMMON NAME	V1C	V1X	T2B	T1C	T1X	T1Y	T4C	T4X	M2C	N2C	P2C	P2X	D2C	D2X	S2C	S2X	L2M	C3C	C1M	C1N	C2N	R1C	R2C	E1C	D2N	B2C	B3C
766	ACETYL ISOBUTYRYL															3												
767	~~DECALIN~~															~~3~~												
768	1,2-DIMETHYLCYCLOHEXENE															3												
769	~~PENTYL TRIMETHYLENE~~															~~3~~												
770	4-METHOXY-1-BUTANOL															3												
771	3,4-EPOXY-3-ETHYL-2-BUTANONE															3												
772	~~2,7-DIMETHYLOCTANE~~															~~3~~					~~3~~							
773	3,4-DIHYDRO-2,5-DIMETHYL-2H-PYRAN-2-CARB															3												
774	~~1,1,3-TRIMETHYLCYCLOHEXANE~~															~~3~~												
775	N-BENZOYLGLYCINE, METHYL ESTER															3												
776	CUMENE ISOPROPYL ETHER															3												
777	2-ISOPROPYL-1,3-DIOXOLANE															3												
778	1-OXIRANYLETHANONE															3												
779	6,6-DIMETHYL-3,4-UNDECADIENE-2,10-DIONE															3												
780	TEREPHTHALIC ACID																3										2	
781	~~XDIMETHYL SULFATE~~																~~3~~					~~2~~						
782	1-METHYL-4-(1-METHYL-2-BUTENYL)NAPHTHALE																3											
783	CYCLOPENTYL BROMIDE																3											
784	2,2-DICHLORO-3-METHYLBUTANE																3				3							
785	X*DIPHENYLAMINE								0		2	0				2	1	2	1	3	2							
786	3-HYDROXY-3-METHYL-2-BUTANONE						3	1	2	3		1	3	2	1	2	0							1				
787	METHYL PENTADECANOATE	1		1			3*																					
788	METHYL PALMITATE	2		2		2*	3*		0*				3*				0*							2*			2*	
789	METHYL ISOPALMITATE	0					3																					
790	DIBENZOFURAN (DIPHENYLENE OXIDE)				1		3					0																
791	2,2-DICHLOROBUTYRIC ACID					2	3								1		2											3
792	2-ETHYLHEPTANOIC ACID						3																				2	
793	4-CHLOROPHENYL ACETATE						3			3																		
794	2,3,4,6-TETRACHLOROPHENOL						3																					
795	1-CHLORO-2-ETHYLBENZENE						3																					
796	PERCHLOROETHANE						3					1																
797	1-BROMO-2-ETHYLBENZENE						3																					
798	CHLOROVINYLBENZENE						3									-1	0				1							
799	$1,2,3-TRICHLOROBENZENE						3																					
800	3,5-DIBROMOTOLUENE						3																					
801	(1,2-DICHLOROETHYL)BENZENE						3														2					1		
802	XM-CHLORONITROBENZENE						3				3								1									
803	*2,4-DICHLORONAPHTHALENE						3																					
804	CYCLOPENTENE						3										2											
805	X+$M-DICHLOROBENZENE						3					0							1		3							
806	X*+$NITROBENZENE						3	-1																				
807	1-CHLOROTRICYCLO[4.3.1.13.8]UNDECANE						3																					
808	DECAMETHYLCYCLOPENTASILOXANE						3				2																	
809	2-CHLORO-1,3,5-TRIMETHYLBENZENE						3																					
810	1-CHLORO-2(PHENYLETHYNYL)BENZENE						3																					

(Continued)

TABLE 11. (Continued)

FINAL REPORT (PART I)

RELATIVE SIZE AND CONCENTRATE WHERE DETECTED

	COMMON NAME	V1C	V1X	T2B	T1C	T1K	T1Y	T4C	T4K	M2C	N2C	P2G	P2X	O2C	O2X	S2C	S2X	L2M	C3C	C1M	C1N	C2N	R1C	R2C	E1G	O2N	B2C	B3C
811	2-METHYLBENZOTRIAZOLE																											
812	XETHYLENE GLYCOL, BIS(2-CHLOROETHYL) ETHE						3																					
813	CYCLODODECANOL						3					3																
814	DIMETHYL SUBERATE						3																					
815	METHYL SUCCINATE,DIMETHYL ESTER						3																					
816	N-METHYL ETHENAMINE						3																					
817	XHEPTANOIC ACID,ETHYL ESTER						3																					
818	2-(2-CHLOROETHOXY)ETHANOL						3																					
819	UNDECANOIC ACID,METHYL ESTER						3																					
820	XBENZENEACETIC ACID,ETHYL ESTER						3																					
821	METHYL P-ETHYLBENZOATE						3							3														
822	XCLOFIBRATE						3																					
823	X9H-FLUOREN-9-ONE						3																					
824	X1-METHYL-2,4-DINITROBENZENE						3									0												
825	2,4-DICHLOROPHENOXY ACETIC ACID, METHYL						3	0																				
826	METHYL ISONONANOATE						3																					
827	XETHYL CAPRYLATE						3																					
828	2-KETOPENTANEDIOIC ACID, DIMETHYL ETHER						3																					
829	CLOFIBRIC ACID,METHYL ESTER						3																					
830	METHYL ISOTRIDECANOATE						3																					
831	ETHYL 7-METHYLMYRISTATE						3																					
832	METHYL PENTACOSANOATE						3																					
833	1-HEXANOL						3																					
834	XHEXYL METHYL KETONE	0				3																						
835	5-HEXEN-2-OL		0			3			1*							2												
836	XN-AMYL ALCOHOL			2	2	3				3																	3	
837	XNICOTINE				3	3		2						2		1								2				2
838	3-METHYL-4-HEPTANONE				2	3		0	2						2		0			3				2				
839	2-DODECANOL					3																						
840	2-HYDROXY-6-METHYLBENZOIC ACID					3																						
841	2-BROMO-1,2-DICHLOROPROPANE				3									3														
842	1-BROMO-2,3-DICHLOROPROPANE				3						3																	2
843	1-(1,3-DIMETHYLBUTOXY)-2-PROPANOL				3						2																	
844	TRIPROPYLENE GLYCOL				3																							
845	X2,6-LUTIDINE				3																			3				
846	X2,4-LUTIDINE				3			1							0				2	3			2	1				
847	2,3-LUTIDENE				3			0				1												1				
848	2,4,6-COLLIDINE				3			0															2	2				
849	3,4,4-TRIMETHYL-2-CYCLOHEXEN-1-ONE				3									1						2			2	2				
850	2-PHENYL ACROLEIN				3										2	2												
851	1-METHYLISOQUINOLINE				3																							
852	2-3-DIMETHYL QUINOLINE				3										3		0											
853	DIDEHYDROGENATED ABIETIC ACID				3										0													
854	X+PHENANTHRENE	0																								1*	3*	3*
855	1,2-BENZISOTHIAZOLE	-1 1	3	1	1*	2*				1*	1*		3*		2*	0*	1*			2*	2*		2*	3* 3*		3*		1*

(Continued)

TABLE 11. (Continued)

FINAL REPORT (PART I)

RELATIVE SIZE AND CONCENTRATE WHERE DETECTED

	COMMON NAME	*	V1C	V1X	T2B	T1C	T1K	T1Y	T4C	T4K	M2C	N2C	P2C	P2X	D2C	D2X	S2C	S2X	L2M	C3C	C1M	C1N	C2N	R1C	R2C	E1C	D2N	B2C	B3C
856	N-PROPYL-1-HEXANAMINE		-1												2							3*							
857	1,2-DIHYDRO-4-PHENYLNAPHTHALENE	a		3										2*		0*													
858	M-DIETHENYLBENZENE	A		3	1					3*						3*													
859	1-PHENYL-3-BUTEN-2-ONE	a		3												2*													
860	BUTYLATED HYDROXY TOLUENE (BHT)			1			1		2			2	1								3	1		2	1		1		1
861	ACETALDEHYDE DIETHYL ACETAL			-1																								3	
862	7-METHYL-3(2H)-BENZOFURANONE			-1																		3	3						
863	NEOPENTYL ALCOHOL				1																				3				
864	3-7,11-TRIMETHYL-3-DODECANOL				3																								
865	2,2#-BI-1,3-DIOXOLANE				3																								
866	N-PROPOXY ETHANOL				3																								
867	ALPHA-PICOLINE					2			3													3							
868	ISOVALERAMIDE					2																		3					
869	$O-CHLOROPHENOL							2													3								
870	$DI-N-PROPYL PHTHALATE								3														3						
871	X+*2,4-DIMETHYLPHENOL (XYLENOL)								0	0																			3
872	PSEUDOCUMENE								0		2	2	1		2		1			3	2	2	1		1				
873	1-INDANONE								2													3							
874	OCTADECANOL								2*																3*		2*		
875	COTININE								1										1						3				
876	TETRAETHYLENE GLYCOL DIMETHYLETHER								0	3									3						2				3
877	1,4,6-TRIMETHYL NAPHTHALENE											2	0												3				
878	MENTHONE												3						3										
879	5-ETHYLDIHYDRO-2(3H)-FURANONE													2							3						1		3
880	VERATRALDEHYDE													3			2								3				
881	TRIETHYLENE GLYCOL, DIMETHYL ETHER													3								3							2
882	4,4-DIMETHYL-2-PENTENOIC ACID														1							3							
883	4-OCTENOIC ACID														2										3				
884	XCHLOROACETONE														3										3				
885	7-NONENOIC ACID															2								3			2		
886	2,6-DIMETHYLHEPTANOIC ACID																1				3		3		2			1	
887	~~2,4-DIMETHYL HEXANE~~																		3										
888	VINYL ACETATE																		3										
889	XMALONIC ACID																			3									
890	4-METHYLPHENYLPENTANOIC ACID																			3									
891	$ISOBUTYL METHYL PHTHALATE																			3									
892	$SEC-BUTYL METHYL PHTHALATE																			3									
893	METHYL METHOXYMETHYL FORMAL																			3									
894	XM-CHLOROANILINE																			3									
895	9-DODECENOIC ACID																				3								
896	2,3,3-TRIMETHYL-3H-INDOLE																				3								
897	2,5-DI-T-AMYL QUINONE																				3	1							
898	XTETRAMETHYLUREA, TMU																				3	2							
899	P-METHYLANISOLE																					2							3
900	ALPHA-METHYL-ALPHA-ACETYLOXYBENZENEACETI																					3							

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TABLE 11. (Continued)

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RELATIVE SIZE AND CONCENTRATE WHERE DETECTED

	COMMON NAME	V 1 C	V 1 X	T 2 B	T 1 C	T 1 X	T 1 Y	T 4 C	T 4 X	M 2 C	N 2 C	P 2 C	P 2 X	O 2 C	O 2 X	S 2 C	S 2 X	L 2 M	C 3 C	C 1 M	C 1 N	C 2 N	R 1 C	R 2 C	E 1 C	D 2 N	B 2 C	B 3 C
901	2,5,8-TRIMETHYL-1-NAPHTHOL																				3							
902	2,5-DIMETHYL STYRENE																				3							
903	1-(3-BUTOXYPROPOXY)-2-PROPANOL (A DIPROP																				3							
904	3-METHYL PHTHALIDE																				3							
905	BUTYL M-TOLYL SULFIDE																				3							
906	TETRAHYDROPYRAN-2-METHANOL																				3							
907	~~3-ETHYL-4-METHYLHEXANE~~																				~~3~~							
908	2-NORBORNENE-7-OL																				3							
909	2-HEXENAL																				3							
910	2,6-DIMETHYL-2-HEPTEN-4-ONE																				3							
911	4-METHYL-3-CYCLOHEXENE-1-CARBOXYLIC ACID																					3						
912	2-ETHYL-2-METHYLBUTYRIC ACID																					3						
913	4-METHYL-2-PHENYLQUINOLINE																					3						
914	1-(PHENYLMETHYL)ISOQUINOLINE																					3						
915	1,2,4-TRIMETHYL-1,3-DIAZOCYCLOHEX-1-ENE																					3						
916	1-ACETYL-1,2,3,4-TETRAHYDROPYRIDINE																					3						
917	VINYL CYCLOHEXYLFORMATE																					2						3
918	DIETHYLENEGLYCOL, CYCLOHEXYL ETHER																					3						
919	ISOINDOLE-1,3-DIONE																						3					
920	2-ETHYL-3-METHYL-2-BUTENEDIOIC ACID																						3					
921	TRICOSANOIC ACID																						2	3				
922	NONACHLOR																						3	2				
923	3-ETHOXY-1(3H)-ISOBENZOFURANONE																						3					
924	2-ISOPROPYLTHIOPHENE																						3					
925	3-(2-HYDROXYPROPYL)-5-METHYL-2-OXAZALIDI																						3	3				
926	3-METHYLOCTAHYDROPENTALENE-1-CARBOXYLIC																							3				
927	4-HYDROXY-OCTAHYDRO-1-NAPHTHALENONE																							3				
928	2,2-DIMETHYL-3-(2-METHYL-1-PROPENYL)CYCL																							3				
929	4-ISOPROPOXYBUTYRIC ACID																							3				
930	DIISOPROPYL PHENOL																							3				
931	ISOSTEARIC ACID																							3				
932	ISOEICOSANOIC ACID																							3				
933	PENTACOSANOIC ACID																							3				
934	HEXACOSANOIC ACID																							3				
935	1,2,4,5,6,7,8,8-OCTACHLORO-2,3,3A,4,7,7A																							3				
936	DIPROPYLENE GLYCOL, 2-PROPENYL ETHER																							3				
937	4-METHOXY-5-METHYL-4-CYCLOPENTEN-1,3-DIO																							3				
938	ISOPROPYL PHENYL PROPAN-1-OL																							3				
939	N-(2-METHYLPHENYL)FORMAMIDE																							3				
940	TETRAPROPYLENE GLYCOL																							3				
941	TETRAPROPYLENE GLYCOL																							3				
942	TETRAPROPYLENE GLYCOL																							3				
943	METHYL DEHYDROABIETATE																							3				
944	1,4-BENZOTHIAZIN-3-ONE																								3	2		
945	8-NONENE-2-ONE																								3*			3*

(Continued)

TABLE 11. (Continued)

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RELATIVE SIZE AND CONCENTRATE WHERE DETECTED

	COMMON NAME	*	V1C	V1X	T2B	T1C	T1X	T1V	T4C	T4X	M2C	N2C	P2C	P2X	D2C	D2K	S2C	S2K	L2M	C3C	C1M	C1N	C2N	R1C	R2C	E1C	D2N	B2C	B3C
946	DODECANEDIOIC ACID																										3		
947	P-BROMOBENZOIC ACID																											3	
948	2,4-DIBROMOBENZOIC ACID																											3	
949	4-PHENYL-4-OXO-BUTYRIC ACID																											3	
950	4(2,5-XYLYL)BUTYRIC ACID																											3	
951	2,5-DI(CHLOROMETHYL)-3-ETHYL BENZOIC ACI																											3	
952	N-ETHYL-4-METHYL-2-PENTANEAMINE																											3	
953	4-ETHYLPHENOL																												3
954	ALPHA-OXOBENZENEACETIC ACID, ETHYL ESTER																												3
955	2-METHOXY-2-HEXENOIC ACID																												3
956	3-DICHLOPOMETHYL-4,6-DI-T-BUTYL-O-BENZOQ																												3
957	CYCLOPENTANE CARBOXYLIC ACID, VINYL ESTE																												3
958	HEXAHYDRO-2H-AZEPINE-2-ONE																												3
959	O-ALLYLTOLUENE	a		1	1					3*				0*	3	3*													
960	P-ETHYL-ISOPROPYLBENZENE	A		1						1*				1*	3							1							
961	M-ETHYLISOPROPYLBENZENE	A		0						0*					3	0*													
962	(1,1-DIMETHYLPROPYL)BENZENE	A		1						1*				2*	3	1*													
963	1-METHYL INDAN			0								2*		1*		3*		0*											
964	1-ETHYL INDAN	A		-1										3*		3*													
965	1-METHYL-1,2-DIPHENYLETHANE	A		1										3*		3*													
966	6-METHYL TETRALIN	A										2		3*		3*													
967	2,3,4-TRIMETHYLBENZOIC ACID												2		3														
968	2-METHYL-2-NONEN-4-ONE												3		3														
969	%CHLOROACETIC ACID													2	2	3		2											1
970	P-DIISOPROPYL BENZENE													2	3		-1												
971	1-HEPTENYLBENZENE													2		3													
972	2,3,6-TRIMETHYL BENZOIC ACID														3														
973	3-METHYL-2,2-DIOXIDE-1H-2,1,3-BENZOTHIAP														3														
974	ISOPROPYL ACETATE														3														
975	.BETA.-OXO-BENZENEACETIC ACID, ETHYL EST														3														
976	1,3-DIHYDRO-2,2-DIOXIDE-2,1,3,BENZOTHIAD														3														
977	METHYLISOBUTYL BENZENE														3														
978	SEC-BUTYL ALCOHOL														3	2													
979	3,5,5-TRIMETHYL-2(5H)-FURANONE														3														
980	2-PROPYLCYCLOHEXANONE														3														
981	5-METHYL-5-PHENYL-2-HEXANONE														3														
982	TETRAMETHYLBENZENE PROPANOIC ACID														3							1							
983	2,2-DIMETHYLPROPANOIC ACID, 2,4,6-TRIMET														3														
984	6-UNDECANONE														3														
985	2,6-DIMETHYLCYCLOHEXANOL														3														
986	HEXAHYDRO-3-(2-PROPENYL)-2H-AZEPIN-2-ONE															3													
987	1(2,6-DIHYDROXY-4-METHOXYPHENYL)ETHANONE															3													
988	%MANDELIC ACID															3													
989	(2-CHLORO-2-PROPENYL)OXYBENZENE															3													
990	DECYL VINYL ETHER	a														3*													

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TABLE 11. (Continued)

FINAL REPORT (PART I)

RELATIVE SIZE AND CONCENTRATE WHERE DETECTED

	COMMON NAME	*	V1C	V1X	T2B	T1C	T1X	T1Y	T4C	T4X	M2C	N2C	P2C	P2X	O2C	O2X	S2C	S2X	L2M	C3C	C1M	C1N	C2N	R1C	R2C	E1C	D2N	B2C	B3C
991	.ALPHA.-HYDROXY-.ALPHA.-METHYL BENZENE A																												
992	4-BUTYL-1,3-CYCLOPENTANEDIONE															3													
993	PHTHIOCOL															3													
994	P-ISOBUTYLTOLUENE															3													
995	%ORCINOL															3													
996	DIBUTYL-3-METHYLGLUTARATE															3													
997	7-METHYL-7-HEPTADECANOL															3													
998	CYCLOHEXYL CHLORIDE										3	2				3	1	2											
999	1-PHENYLNAPHTHALENE	A		2										3*		0*													
1000	2-PHENYLNAPHTHALENE	A		1										3*															
1001	2-ETHYL TETRALIN	A		1						2*				3*		2*													
1002	%2-METHYLANTHRAQUINONE	a		1										3*															
1003	4-METHYL INDAN	A		-1	1					3*				3*			0												
1004	BENZILIDENEACETONE	A		0										3*		2*													
1005	2,4-DIMETHYL-1-SEC-BUTYLBENZENE	A								2*				3*	2	2*													
1006	4-ETHYLBENZYL ALCOHOL	a												3*		2*													
1007	1,3-DIMETHYNAPHTHALENE	a												3*								2			1				
1008	(2-METHYL-1-PROPENYL)BENZENE	A												3*	1	2*		0*											
1009	P-DIPROPYLBENZENE	A												3*															
1010	(1,1-DIMETHYLBUTYL) BENZENE	A												3*		2*													
1011	%AZULENE	a												3*				1*											
1012	1-METHYLFLUORENE	a												3*											1				
1013	3,5,5-TRIMETHYL-2-CYCLOPENTEN-1-ONE													3		1													
1014	OCTAHYDROINDENE	a												3*				0*											
1015	%$O-XYLENE				2				1				3				2	2					1						1
1016	BUTYL FORMATE				2								3																
1017	IODOCYCLOHEXANE										3	2	3		2		0												
1018	2,2-DIMETHYLSUCCINIC ACID												3																
1019	TRANS-3-BUTYLTETRAHYDRO-2-METHYLFURAN												3																
1020	4-HYDROXY-3-METHYL-2-(2-PROPENYL)-2-CYCL												3																
1021	OCTAHYDRO-4A,5-DIMETHYL-3-ISOPROPYL-2(1H												3																
1022	2,4-DIMETHYL-2-PENTANOL												3																
1023	D-FENCHONE												3				-1												
1024	1,2-DIMETHYL-3-ISOPROPENYLCYCLOPENTANOL												3																
1025	4,8-DIMETHYL-7-NONEN-2-ONE												3				2												
1026	2-METHYL-1-PENTEN-3-ONE												3																
1027	2,2-DIMETHYL-3,5-DECADIENE												3																
1028	2,4,6-TRICHLOROANILINE		-1			2			2*			3*	2*				0*	1		1*		1*			2*			0*	
1029	2,4-DIMETHYL HEXANOIC ACID							1				3																	
1030	1-ETHYL-3-METHYL BENZENE							1				3			2					2	1								
1031	1,6 DIMETHYL-4-ISOPROPYL-NAPHTHALENE								1		1	3	2		1		0		2	1		2			2		1		
1032	1,2,3-TRIMETHYL BENZENE								0		2	3	2	0			1			2	2	1			0				
1033	1-(3,3-DIMETHYLOXIRANYL)ETHANONE								2			3					2												
1034	4,4-DIMETHYL-1,3-DIOXANE											3																	
1035	%3,4-DICHLOROPHENOXYACETIC ACID											3																	

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TABLE 11. (Continued)

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RELATIVE SIZE AND CONCENTRATE WHERE DETECTED

	COMMON NAME	* V1C	V1X	T2B	T1C	T1X	T1Y	T4C	T4X	M2C	N2C	P2C	P2X	O2C	O2X	S2C	S2X	L2N	C3C	C1M	C1N	C2N	R1C	R2C	E1C	D2N	B2C	B3C
1036	DODECAMETHYLCYCLOHEXASILOXANE										3					0												
1037	%2,6-DIMETHYLNAPHTHALENE										3								2	2								
1038	%O-CHLORONITROBENZENE										3													2				
1039	%MESITYLENE										3	2				0	2		2		2							0
1040	1-(DICHLOROMETHYL)-4-ETHYLBENZENE										3																	
1041	1,1-DIBUTOXY-BUTANE										3																	
1042	CIS-9-OCTADECENAMIDE										3																	
1043	%*TRIPHENYL PHOSPHATE										3													1				
1044	3,3,5-TRIMETHYCYCLOHEXANONE										3																	
1045	4-ISOPROPYLACETOPHENONE										3					1												
1046	2-METHYL-3-OXOHEXANOIC ACID, ETHYL ESTER										3																	
1047	DIAMYLPHTHALATE										3																	
1048	4,7,7-TRIMETHYLBICYCLO(2.2.1)HEPTAN-2-ON										3																	
1049	%*O-CHLOROTOLUENE						1	0		3						-1	0							1	1			
1050	1,1,2,3-TETRACHLOROPROPANE							0*		3	2*	1*				0*	2									1*		
1051	ETHYL BUTYL KETONE							1		3					2	1	1					2		1				
1052	%M-AMINOACETOPHENONE								2	3																		
1053	ALPHA-CHLOROPROPIONIC ACID									3																		
1054	2,3-DIMETHYL-2-PENTANOL									3																		
1055	3-CHLORO-2-METHYL-1-BUTENE									3																		
1056	2,3-DICHLOROISOBUTANAL									3																		
1057	1-CHLORO-3-(CHLOROMETHYL)BENZENE									3																		
1058	1,4-DIHYDRO-1-METHYL-4-OXONICOTINONITRIL									3																		
1059	2,4,4-TRIMETHYL-2-PENTENAL									3																		
1060	1-METHYL-4-ISOPROPYL-1,2-CYCLOHEXANEDIOL									3																		
1061	%3-METHYL-1-BUTANOL ACETATE									3						1												
1062	TIGALDEHYDE									3		1				1												
1063	TRIMETHYLOXIRANE									3						2												
1064	1-HYDROXY-3-METHYL-2-BUTANONE									3																		
1065	CIS-2,3-EPOXYHEXANE									3																		
1066	2,4-DIMETHYLPENTANAL									3						1												
1067	CYCLOHEXYL ETHER									3																		
1068	3-ETHYL-2,2-DIMETHYLOXIRANE									3						2												
1069	4-HYDROXY-3-METHYL-2-BUTANONE									3																		
1070	TRANS,CIS-4,5-DIETHYL-3,5-OCTADIENE									3																		
1071	3-HYDROXYBENZALDEHYDE		-1						3																			
1072	2,2-DIETHOXYETHANOL		0						3*																			
1073	6-ETHYL TETRALIN		0						3*				2*		2*													
1074	2-HYDROXY-3,5,5-TRIMETHYL-2-CYCLOHEXENE. A					2		2	3																			
1075	3,3-DICHLORO-2-PROPENOIC ACID						2		3			2			2													
1076	3-HYDROXYCAPRIC ACID							3																				
1077	1-ALLYLNAPHTHALENE							0	3										1		1							
1078	2-METHYLFURAN							3								2												
1079	N-PHENYL ACETAMIDE							3	3																			
1080	N,N-DIMETHYLBENZYLAMINE							3	2						2									2				

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TABLE 11. (Continued)

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RELATIVE SIZE AND CONCENTRATE WHERE DETECTED

	COMMON NAME	V1C	V1X	T2B	T1C	T1X	T1Y	T4C	T4X	M2C	N2C	P2C	P2X	D2C	D2X	S2C	S2X	L2M	C3C	C1M	C1N	C2N	R1C	R2C	E1C	D2N	B2C	B3C
1081	TETRAPROPYLENE GLYCOL METHYL ETHER							3										2										
1082	4-CHLOROCROTONIC ACID								3				1															1
1083	M-DI-SEC-BUTYLBENZENE								3																			
1084	P-DI-SEC-BUTYLBENZENE								3																			
1085	X2-METHYL-2-PHENYLOXIRANE								3																			
1086	6,6-DIMETHYL-2,5,10-UNDECANETRIONE								3							2												
1087	2-METHYL-2-CYCLOPENTEN-1-ONE								3					2		2	1											
1088	3,4-DIMETHYLBENZALDEHYDE								3						2													
1089	$ETHYLBENZENE			2				2*						2*		2*	2*	2*				1*						1*
1090	3-BROMOHEPTANE						2																					
1091	N-BENZOYL-L-ALANINE, METHYL ESTER	1														2												
1092	1,1,2-TRICHLORO-1-PROPENE				1					2	2						2											
1093	2-ETHYLACETOACETIC ACID												1	2		2												
1094	5-METHYL-3-HEXEN-2-ONE													2		2												
1095	4,4-DIMETHYLHEXANAL														1	2												
1096	TETRAHYDRO-2H-PYRAN-2-ONE															2												
1097	2-DECANOL															2												
1098	2,5-DICHLORO-4-METHYLBENZOIC ACID															2												
1099	1-NAPHTHOIC ACID															2												2
1100	2-CHLORO-3-METHYL-2-BUTENE															2												
1101	*+$PENTACHLOROBIPHENYL + OTHER PCBS															1	2							1				
1102	2,4-DICHLOROPENTANE															2												
1103	3,6-DIMETHYL-3-HEPTANOL															2												
1104	1-ETHOXY-2-HEPTANONE															2												
1105	3-CYCLOHEXYL-4-PENTEN-2-ONE															2					1							
1106	3-METHYL-1,2,4-CYCLOPENTANETRIONE															2												
1107	3-ETHOXYPROPANAL															2												
1108	1-(1-CYCLOHEPTEN-1-YL)ETHANONE															2												
1109	4,4,5,5-TETRAMETHYL-2,7-OCTANEDIONE															2												
1110	XBETA-CITRONELLOL															2												
1111	3-ETHYL-4-METHYL-3-PENTEN-2-ONE															2												
1112	4,4-DIMETHYLCYCLOHEXENE															2												
1113	1-NITRO-2-OCTANONE															2												
1114	~~2,3,3-TRIMETHYLHEXANE~~															2												
1115	5,5-DIETHOXY-3-PENTYN-2-ONE															2												
1116	3-ALLYL-2,4-PENTANEDIONE															2												
1117	2,2-DIMETHYL-3-PROPYLOXIRANE															2												
1118	7-METHYL-3-OCTEN-2-ONE															2												
1119	MENTHYL ACETATE															2												
1120	3-METHYL-3-DECEN-2-ONE															2												
1121	DI-SEC-BUTOXYMETHANE															2												
1122	XANTHENE															2												
1123	6-DODECANOL															2												
1124	2-METHYL-2-HEXANOL															2												
1125	5-METHYL-3-METHYLENE-2-HEXANONE															2												

(Continued)

TABLE 11. (Continued)

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RELATIVE SIZE AND CONCENTRATE WHERE DETECTED

	COMMON NAME	V1C	V1X	T2B	T1C	T1K	T1Y	T4C	T4X	M2C	N2C	P2C	P2X	O2C	O2X	S2C	S2X	L2N	C3C	C1M	C1N	C2N	R1C	R2C	E1C	D2N	B2C	B3C
1126	CYCLODECANOL															2												
1127	1-(ETHNYLOXY)PENTANE															2												
1128	CIS-3,4-DIMETHYL-3-HEXEN-2-ONE															2												
1129	PHENYLBUTANAL															2												
1130	CIS-5-BUTYLDIHYDRO-4-METHYL-2(3H)-FURANO															2												
1131	2,6-DIISOPROPYLPHENOL															2	2											
1132	ALPHA-FARNESAL															2												
1133	3A,4,5,7A-TETRAHYDRO-4-HYDROXY-3A,7A-DIM															2												
1134	BUTYL CYANATE															2												
1135	ETHYL AMYL KETONE															2												
1136	3,8-NONADIEN-2-ONE															2												
1137	3A,4,7,7A-TETRAHYDRO-2-PROPYL-1H-ISOINDO															2												
1138	2-HEXEN-1-OL															2												
1139	ISOCYANOETHANE															2												
1140	4-PENTEN-2-OL															2								2				
1141	3-CHLORO-3-BUTEN-2-ONE															2												
1142	[2-(PENTYLOXY)ETHYL]CYCLOHEXANE															2												
1143	2,4-DI-TERT-BUTYLPHENOL															2												
1144	2-CHLORO-2-PROPENOIC ACID																2											
1145	BETA-RESORCYLIC ACID																2											
1146	P-NITROBENZOIC ACID																2											
1147	~~HEPTANE~~																2				1							
1148	TETRAHYDROFURFURYL ALCOHOL; THFA																2											
1149	LOLIOLIDE																2											
1150	%*+$FLUORANTHENE	-2					2	0*	0	1*			1				-1			1*				2*				1*
1151	METHYL HEPTADECANOATE	-1					2																					
1152	%PROPIOPHENONE		0				2								1													
1153	(1-NITROETHYL)BENZENE		1				2																					
1154	2,3,4,5-TETRACHLOROANILINE				1		2			1																		
1155	2-METHYL-1-NAPHTHALENOL						2																					
1156	2,3-DICHLOROBUTENE						2																					
1157	1-BROMO-2-CHLORO-2-BUTENE						2																					
1158	2,4-DICHLORO-1-(CHLOROMETHYL)BENZENE						2																					
1159	1,2-DICHLORO-4-(CHLOROMETHYL)BENZENE						2																					
1160	%+9H-FLUORENE						2												1				2	2				2
1161	P-BROMOTOLUENE						2																					
1162	1,2-DICHLORO-3-NITROBENZENE						2										1											
1163	2-CHLORO-P-CYMENE						2																					
1164	2-CHLORO-1-(4-ETHYLPHENYL)-2-METHYL-1-PR						2								0													
1165	+%*$LINDANE						2				2					1	0							1				
1166	METHYL DICHLOROACETATE						2									1												2
1167	%URETHANE (ETHYLCARBAMATE)						2		1						2													
1168	4-CHLOROPHENYL ACETIC ACID, METHYL ESTER						2																					
1169	METHYL ANTEISOPENTADECANOATE						2																					
1170	P-CHLORO-2-NITROANILINE						2																					

(Continued)

TABLE 11. (Continued)

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RELATIVE SIZE AND CONCENTRATE WHERE DETECTED

	COMMON NAME	*	V1C	V1X	T2B	T1C	T1K	T1Y	T4C	T4X	M2C	N2C	P2C	P2X	D2C	Q2K	S2C	S2X	L2M	C3C	C1M	C1N	C2N	R1C	R2C	E1C	D2N	B2C	B3C
1171	2,4-D, ETHYL ESTER																												
1172	ALPHA-KETOGLUTARIC ACID							2																					
1173	METHYL PROPENYLOXY KETONE						2																						
1174	3,4,5-TRIMETHYL-2-CYCLOPENTEN-1-ONE					2																							
1175	%ETHYLENE GLYCOL					2									2	2													1
1176	GAMMA-PICOLINE					2														2									
1177	2,5-LUTIDINE					2			0																				
1178	2,3,6-TRIMETHYLPYRIDINE					2																			1				
1179	5-ETHYL-2-PICOLINE					2																			1				
1180	2,3,4-TRIMETHYLPYRIDINE					2																							
1181	2,4,5-COLLIDINE					2																							
1182	2-ETHYL-6-PICOLINE					2																			1				
1183	4,4,5-TRIMETHYL-2-CYCLOHEXEN-1-ONE					2																							
1184	%QUINOLINE					2																							
1185	%QUINALDINE					2																			2				1
1186	DIPROPYLENE GLYCOL					2			1																1				
1187	2-(1-METHYL-2-PIPERIDINYL)-PYRIDINE					2				1																			
1188	ABIETIC ACID					2																							
1189	METHYLOCTADEC-10-ENOATE		0																									2*	
1190	METHYL-9,11-OCTADECADIENOATE		0		2																								
1191	M-METHOXYPHENYL ACETATE		1		2																								
1192	2-METHYL TETRALIN			0															2										
1193	4-METHYLPHENANTHRENE	A		2										2*		1*													
1194	3-METHYL INDENE			1										2*											2				
1195	DIMETHYL NAPHTHALENE	A		2																									
1196	3-ETHOXYPROPIONITRILE	A		2																1	2								
1197	(2-PHENYLETHYL)ACETATE			2																									
1198	2-XYLYLETHANOL			2																									
1199	ACETYL BIPHENYL			2																									
1200	4-OCTANONE			2													-1												
1201	3-BUTEN-2-OL			2												1*													
1202	0-ETHYLSTYRENE				2																								
1203	1-HEPTADECENE	A			2					2*		1													1				
1204	3,5-DIMETHYL-2-CYCLOHEXEN-1-ONE				2																								
1205	DODECANAMIDE				2					2						1		0											
1206	METHYL-2,3-DIMETHYL BENZOATE				2											2													
1207	METHYL-11-OCTADECENOATE				2																								
1208	METHYL-9,12,15-OCTADECATRIENOATE				2																								
1209	%N,4-DIMETHYLBENZENESULFONAMIDE				2																								
1210	3-METHYL-1-PENTANOL				2																			2					
1211	%P-CYMENE (P-ISOPROPYL TOLUENE)				2																								
1212	4-PHENYL PENTANOIC ACID					1							2	0								2							
1213	COUMARONE								2										2										
1214	%PHENYL ETHER								0													2							
1215	*2-METHYL STYRENE								2			2	1											1	2				
									0				0				-1		1	1	2	1	1		1				

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TABLE 11. (Continued)

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RELATIVE SIZE AND CONCENTRATE WHERE DETECTED

	COMMON NAME	V1C	V1X	T2B	T1C	T1X	T1V	T4C	T4X	M2C	N2C	P2C	P2X	O2C	O2X	S2C	S2X	L2M	C3D	C1M	C1N	C2N	R1C	R2C	E1C	D2N	B2C	B3C
1216	3,5,5-TRIMETHYLCYCLOHEX-3-EN-1-ONE								1					1	1			2										
1217	2,3,4-TRIMETHYL-2-CYCLOPENTEN-1-ONE								1						2													2
1218	1,6-DIMETHYLNAPHTHALENE										2	2		0		-1				1			1	2				
1219	4-PHENYLBICYCLOHEXYL										2					1							2	1				
1220	%*+$HEXACHLOROBENZENE										1	0									2	1		1				
1221	%3,5-DICHLOROPHENOL											2															2	
1222	O-ETHYL TOLUENE											2	0			1			2	2	2							
1223	4,7-DIMETHYLBENZOFURAN											0									2							
1224	1,3,6-TRIMETHYLNAPHTHALENE											0								2	1							
1225	6-METHYL-3,5-HEPTADIEN-2-ONE													2														2
1226	2-METHYLCYCLOPENTANONE													2*	1*			2*			2*							2*
1227	1-ACETYLPIPERIDINE														2							2						
1228	5-ETHENYL TETRAHYDRO-.ALPHA.,.ALPHA.,5-T														2													2
1229	2,4,5,7-TETRAMETHYLPHENANTHRENE															-1					2							
1230	DIPROPYL CARBINOL																1					2						2
1231	%GUAIACOL																1					2						
1232	8-NONENOIC ACID																	2										
1233	METHOXYNAPHTHALENE																	2										
1234	3,3,4-TRIMETHYLDECANE																	2										
1235	2-OCTYLPHENOL																		2									
1236	1,3,5-TRICHLORO-2-METHOXYBENZENE																		2				2					
1237	DIMETHYLNAPHTHALENE																		2									
1238	METHYL 4-BUTOXYBUTYRATE																		2									
1239	*TRI-M-CRESYLPHOSPHATE																		2									
1240	2-AMINO-5-PICOLINE																			2								
1241	TRANS-2-ETHYL-3-PROPYLOXIRANE																				2							
1242	PENTACHLOROPYRIDINE																				2	2						
1243	2,3,4-TRIMETHYLOXETANE																				2							
1244	2,5-DIMETHYL THF																				2							
1245	4-BROMO-3-PHENYLSYDNONE																				2							
1246	3,8-DIMETHYL-5-ISOPROPYL-1,2-NAPHTHOQUIN																				2							
1247	CHLOROIODOMETHANE																				2							
1248	1-METHYL-4-(1-METHYLETHENYL)-CYCLOHEXENE																				2					0		
1249	1-(2-BROMOETHYL)-4-CHLOROBENZENE																				2			1				
1250	3,4,5,6-TETRAMETHYLPHENANTHRENE																				2							
1251	(2-BROMOCYCLOPROPYL)BENZENE																				2							
1252	OCTAHYDROAZOCINE																				2							
1253	PIPERIDONE																				2							
1254	P-TOLYL ACRYLIC ACID																				2							
1255	N-HEXYLBUTANAMIDE																				2							
1256	4H-PYRAN-4-ONE																				2							
1257	2-CYCLOHEXENOL																				2	2					2	
1258	5-DECANONE																				2							
1259	3,3-DIMETHYL-2-HEXANONE																				2							
1260	4-METHYLHEXANAL																				2							2

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TABLE 11. (Continued)

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RELATIVE SIZE AND CONCENTRATE WHERE DETECTED

	COMMON NAME	*	V1G	V1X	T2B	T1C	T1X	T1Y	T4C	T4X	M2C	N2C	P2C	P2X	D2C	D2X	S2C	S2X	L2M	C3C	C1M	C1V	C2N	R1C	R2C	E1C	D2N	B2C	B3C
1261	1-VALERYLPYRROLIDINE																						2						
1262	1-ETHYL-2,5-PYRROLIDINEDIONE																						2						
1263	CONIINE																						2						
1264	HEPTYL ACETATE																						2						
1265	~~PHOSPHORIC ACID~~																							~~2~~					
1266	2-ETHYLVALERIC ACID																							2					2
1267	1,5-DIPHENYL-3-PENTANONE																							2					
1268	OCTAHYDROPHENANTHRENE CARBOXALDEHYDE																							2	2				
1269	4,6-DIMETHYLNONANOIC ACID																								2				
1270	DIMETHYLFLUORENE																								2				
1271	1,2,3,4-TETRACHLOROBUTANE																								2				
1272	2,2-DIMETHYL-1,3-CYCLOPENTANEDIONE																								2				
1273	5-DODECANONE																								2				
1274	X2,6-DIMETHYLQUINOLINE																								2				
1275	TETRAPROPYLENE GLYCOL																								2				
1276	N-ETHYL-2-BENZOTHIAZOLAMINE																								2				
1277	DIMETHYLCYCLOHEXANE DIONE																								2				2
1278	2,2,4-TRIMETHYL-1,3-PENTANEDIOL																								2				
1279	2,2,5,7-TETRAMETHYL-4,5-OCTADIENE-3-ONE																								2				
1280	1,2-DIAZABICYCLO[2.2.2.]OCTAN-3-ONE																									2			
1281	2-METHOXY-10-UNDECENOIC ACID																										2		
1282	CETENE																										2		
1283	1-OCTADECENE																										2		
1284	1-PROPOXY-2-PROPANOL																											2	
1285	5-METHYL-5-ETHYL-2,4-OXAZOLIDINEDIONE																											2	
1286	BROMOCHLOROBENZOIC ACID																											2	
1287	16-HYDROXY PALMITIC ACID																											2	
1288	P-AMINOBENZENE-T-BUTYRIC ACID																												2
1289	BARBITAL																												2
1290	TRIMETHYL-6-VINYLTETRAHYDROPYRAN-3-OL																												2
1291	5,5-DIMETHYLFURANONE																												2
1292	5-HEPTEN-2-ONE																												2
1293	N-METHYL-2-PIPERIDINONE																												2
1294	3,4-DIMETHYL-3-PENTEN-2-ONE																												2
1295	PHENYLCYCLOHEXANE	A		1						2*				2*		2*													
1296	ETHYLVALERATE			0											2														
1297	XETHYL HEXANOATE			0											2														
1298	1-(1-ETHYLPROPYL)-2-PROPYLBENZENE	A		-1						2*				2*		2*													
1299	SYM-DIPHENYLETHANE (BIBENZYL)	A		1												2*													
1300	DIETHYL TOLUENE	A		1	1							1			2														
1301	1,6-DIMETHYL DECALIN				1										2														
1302	XM-TOLUQUINONE					1										2													
1303	4-METHYLCYCLOHEXANE CARBOXYLIC ACID								1						2														
1304	1,4-DIMETHYL-2-ISOBUTYL BENZENE	A								0*						2*													
1305	5-METHYLFURFURAL									1					2														

* SEE FOOTNOTE ON LAST PAGE

(Continued)

TABLE 11. (Continued)

FINAL REPORT (PART I)

RELATIVE SIZE AND CONCENTRATE WHERE DETECTED

	COMMON NAME	*	V1C	V1X	T2B	T1C	T1X	T1Y	T4C	T4X	M2C	N2C	P2C	P2X	O2C	O2X	S2C	S2X	L2M	C3C	C1M	C1N	C2N	R1C	R2C	E1C	D2N	B2C	B3C
1306	1,1-DIMETHYL INDENE												1		2		-1												
1307	2-PENTENOIC ACID													2		2													
1308	CLOFIBRIC ACID, M-CHLORO ISOMER														2														
1309	7-OXO-OCTANOIC ACID														2												1		
1310	1,2,3,3A-TETRAHYDRO AZULENE														2														
1311	~~2,6-DIMETHYLOCTANE~~														2														
1312	6-METHYL-BICYCLO(4.1.0)HEPTANONE														2														
1313	XFURFURAL														2														
1314	2-METHYL-2-(1-METHYLPROPYL)-OXIRANE														2														
1315	XDIETHYL SULFITE														2														
1316	~~1,2,4-TRIMETHYL-CYCLOHEXANE~~														2														
1317	3-ISOPROPYL-2,4-PENTANEDIONE														2														
1318	2-METHLY-5-ISOPROPYLCYCLOHEXANONE														2														
1319	2-BUTYL-2-OCTENAL														2														
1320	3,3-DIMETHYL-2(3H)-FURANONE														2														
1321	3-HYDROXY-2,4-PENTANEDIONE,BENZOATE														2														
1322	2,2-DIMETHYLHEXANEDIOIC ACID, DIMETHYL E														2														
1323	VINYL CHLORIDE															2													
1324	XCROTONIC ACID															2													
1325	3-PENTENOIC ACID															2													
1326	XOXALIC ACID															2													
1327	1-ETHYL-2,3-DIMETHYL BENZENE															2													
1328	(1-ETHYL-2-PROPENYL)-BENZENE															2													
1329	2,6-DIMETHYLSTYRENE															2													
1330	BIS(3-METHYLPHENYL)METHANONE															2													
1331	CIS-2,3-DIHYDRO-2-METHYL-1H-INDENE-1,2-D															2													
1332	2,3-DIHYDRO-3,3-DIMETHYL-1H-INDEN-1-OL															2	0												
1333	1-(1-CYCLOHEXEN-1-YL)ETHANONE															2													
1334	M-MENTH-1(7)-ENE (R)-(-)															2													
1335	1,7,DIHYDRO-2-(METHYLAMINO)-6H-PURIN-6ON															2													
1336	1-ALLYLBENZENE															2													
1337	2(3H)-BENZOTHIAZOLONE															2			1										
1338	XP-TOLUQUINONE															2													
1339	3',4'-DIHYDROXYACETOPHENONE												2*																
1340	TRANS-3-METHYL-3-PENTENOIC ACID												2																
1341	O-CRESOTIC ACID												2				1												
1342	PHLOROL												2																
1343	2,3-DIMETHYL TETRALIN												2																
1344	OCTYL BENZENE												2			-1													
1345	2,4,5-TRIMETHYLBENZALDEHYDE												2				0												
1346	3-METHYLSTILBENE	0											2*																
1347	2-METHYL-3-HEXANOL												2				-1												
1348	BENZIL												2																
1349	2-(1-(2-METHOXYETHOXY)ETHOXY)ETHANOL												2																
1350	1,1,2,3,3-PENTACHLOROPROPANE							0		2	2	2				0	1						1						

* SEE FOOTNOTE ON LAST PAGE

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TABLE 11. (Continued)

FINAL REPORT (PART I)

RELATIVE SIZE AND CONCENTRATE WHERE DETECTED

	COMMON NAME	*	V1G	V1X	T2B	T1G	F1X	T1Y	T4G	T4X	M2G	N2G	P2G	P2X	O2G	O2X	S2G	S2X	L2W	G3G	C1M	C1N	C2N	R1G	R2G	C1G	O2W	B2C	B3C
1351	5-METHYL TETRALIN											1	2	0															
1352	2-PROPYLHEPTANOIC ACID												2																
1353	O-ISOPROPYLBENZOIC ACID												2																
1354	1-METHYL-2-CYCLOHEXEN-1-OL												2																
1355	4-ETHYLPYRIDINE												2																
1356	X1,3,6-TRIMETHYL-2,4(1H,3H)-PYRIMIDINEDIO												2																
1357	XCAPRALDEHYDE												2																
1358	3*,4*-DIMETHOXYACETOPHENONE												2				0												
1359	2-METHYL-3-PENTANONE											2																	
1360	2-ETHYL PENTANOIC ACID											2																	
1361	~~UNDECANE~~											~~2~~															~~1~~		
1362	1-ETHYL-3,5-DIMETHYL BENZENE											2	1			1				1									
1363	4-ETHYL-1,2-DIMETHYL BENZENE											2	1					0		1									
1364	ISODURENE											2					-1			1									
1365	1,2-DIMETHYL INDAN											2	1																
1366	X1,4-DIMETHYLNAPHTHALENE											2																	
1367	P-CHLORONITROBENZENE											2																	
1368	2,3,6-TRIMETHYLNAPHTHALENE											2	0				-1				1	1			1				
1369	1,6,7-TRIMETHYLNAPHTHALENE											2	1								1	1							
1370	5-CHLORO-2-METHYLBENZOFURAN											2																	
1371	CIS-1,2,3-TRIMETHYL-4-PROPENYLNAPHTHALEN											2																	
1372	CHLOROFLUOROBENZENE											2																	
1373	1,1,3-TRICHLORO-2-METHYL-1-PROPENE											2																	
1374	PENTACHLOROBENZENE											2																	
1375	2-T-BUTYL NAPHTHALENE											2																	
1376	~~DECYLCYCLOHEXANE~~											~~2~~																	
1377	X* +$HEPTACHLOR											2													1				
1378	NITROCYCLOHEXANE											2																	
1379	2,6-DIMETHYLCYCLOHEXANONE											2																	
1380	METHOXYCYCLOHEXANE										2																		
1381	P-ETHYL TOLUENE										2				0														
1382	ACETOIN										2						1												
1383	2-METHYL-2-ISOPROPYL-1,3-DIOXOLANE										2																		
1384	DIMETHYL ISOPROPYL BENZENE								2																				
1385	2,2*METHYLENEBIS(6-(1,1-DIMETHYLETHYL)-4								2																				
1386	DIMETHYL INDAN									2																			
1387	2,4,6-TRIMETHYLBENZALDEHYDE	a								2*					1			0											
1388	M-ANISALDEHYDE									2																			
1389	DIBROMOCYCLOHEXENE									2																			
1390	META-CYMENE (M-ISOPROPYL TOLUENE)													0			1				1								
1391	2-KETO-3-METHYL VALERIC ACID																1												
1392	5-HEXENOIC ACID																1												
1393	3,3-DIMETHYLBUTYNE																1												
1394	SEC-ISOAMYL ALCOHOL																1												1
1395	7-OCTEN-4-OL																1												

* SEE FOOTNOTE ON LAST PAGE

(Continued)

TABLE 11. (Continued)

FINAL REPORT (PART I)

RELATIVE SIZE AND CONCENTRATE WHERE DETECTED

	COMMON NAME	*	V 1 C	V 1 X	T 2 B	T 1 C	T 1 X	T 1 Y	T 4 C	T 4 X	M 2 C	N 2 C	P 2 C	P 2 X	O 2 C	O 2 X	S 2 C	S 2 X	L 2 M	C 3 C	C 1 M	C 1 N	C 2 N	R 1 C	R 2 C	E 1 C	D 2 N	B 2 C	B 3 C
1396	2-METHYLCYCLOPENTANOL ACETATE																1												
1397	2,4-DIISOPROPYLPHENOL																1												1
1398	ETHYL 4-HYDROXYPHENYLACETATE																1												
1399	TRIETHYLENE GLYCOL, PHENYL ETHER																1												
1400	2-ETHYL-3-PROPYLOXIRANE																1												
1401	DMU (DIMETHYL UREA)																1												
1402	P-(1-ETHYLPROPYL)TOLUENE																1												
1403	2-METHYL-1-DODECANOL																1												
1404	2-METHYLENE-1-BUTANOL ACETATE																1												
1405	TETRAHYDROFURFURYL ACETATE																1												
1406	5-METHOXY-2-PENTANONE																1												
1407	5-(ACETYLOXY)-2-PENTANONE																1												1
1408	PINACOL																1												
1409	1,1-DIMETHOXYCYCLOHEXANE																1												
1410	METHYL 3,6-DIHYDRO-4,5-DIMETHYL-2H-PYRAN																1												
1411	5-NONANOL																1												
1412	1-TERT-BUTOXY-2-METHYLCYCLOHEXENE																1												
1413	O-ISOPROPYLACETOPHENONE																1												
1414	NONYLPHENOL																1												
1415	%2-FUROIC ACID																	1											
1416	CROTONYLBENZENE																	1											
1417	ALLYLACETONE																	1											
1418	SPIRODODECANE																	1											
1419	1-PHENYL-1,2-PROPANEDIONE																	1											
1420	1-(BROMOMETHYL)-4-METHYLBENZENE						1																						
1421	P-CHLOROANISOLE						1																						
1422	1,2,4,5-TETRACHLOROBENZENE						1																						
1423	(1-CHLOROETHYL)DIMETHYLBENZENE						1																						
1424	2-BROMO-4-METHYL-1-ISOPROPYLBENZENE						1																						
1425	1-(CHLOROMETHYL)NAPHTHALENE						1																						
1426	*$TETRACHLOROBIPHENYL						1																	1					
1427	*$PENTACHLOROBIPHENYL						1																						
1428	3-HEXYL BROMIDE						1					1																	
1429	1,1,2-TRICHLOROPROPANE				1											-1													
1430	5,8-DIMETHYLQUINOLINE				1																								
1431	2,3,5-COLLIDINE				1																			1					
1432	4-ETHYL-2,6-DIMETHYL PYRIDINE				1																			1					
1433	3-ETHYL-2,4,5-TRIMETHYL-1H-PYRROLE				1																								
1434	%2,4-DIMETHYLQUINOLINE				1																								
1435	METHYL OLEATE		1																										
1436	9,12-OCTADECADIENOIC ACID		1																										
1437	4-ETHENYL BENZOIC ACID	A		1																									
1438	4-HYDROXYACETOPHENONE			1																									
1439	1-NAPHTHALENOL			1																									
1440	DIETHYL PHENOL,(UNKNOWN ISOMER)			1																									

* SEE FOOTNOTE ON LAST PAGE

(Continued)

TABLE 11. (Continued)

FINAL REPORT (PART I)

RELATIVE SIZE AND CONCENTRATE WHERE DETECTED

	COMMON NAME	*	V1C	V1X	T2B	T1C	T1X	T1Y	T4C	T4X	M2C	N2C	P2C	P2X	D2C	Q2X	S2C	S2X	L2N	C3C	C1M	C1N	C2N	R1C	R2C	E1C	D2N	B2C	B3C
1441	METHOXYBENZENE			1																									
1442	2,2-DIMETHYL-1,1-BIPHENYL	A		1																									
1443	ALPHA-HYDROXY-ALPHA-PHENYL PHENYL ACETIC			1																									
1444	1-METHYL ANTHRACENE			1																									
1445	4-METHYL-3-HEPTANONE			1													-1												
1446	METHYL PROPIONATE			1																									
1447	P-METHYL ACETOPHENONE	a		1																									
1448	2#,4#,6#-TRIMETHYLACETOPHENONE	a		1																									
1449	1-T-BUTYL-3-ETHYL-5-METHYL BENZENE	A		1																									
1450	2-ALLYL BENZOATE	a		1																									
1451	1-METHOXYETHYLBENZENE	a		1																									
1452	QUINOXALINE			1																									
1453	ETHYL MARGARATE	A		1									1*																
1454	BENZOPHENONE	a		1																									
1455	%+PYRENE		0		1									1*							1*								
1456	7-ETHYLQUINOLINE			0																		1							
1457	2-ETHOXYBUTANE				1																								
1458	HYDROGENATED ABIETIC ACID				1																								
1459	1-ETHYL-METHYLCYCLOPENTANE				1																								
1460	%$CUMENE				1				-1				1		1					1									
1461	BENZALDEHYDEOXIME				1																								
1462	METHYL PALMITOLEATE				1																								
1463	%+ACENAPHTHALENE								0								-1				1*				1*		0*		0*
1464	1-METHYL-4-PROPYLBENZENE										1						-1					1							
1465	%+$DDE											1		1											1				
1466	2-ETHYL-1,4-DIMETHYL BENZENE												0				-1			1									
1467	1,2,8-TRIMETHYLNAPHTHALENE (3,4,5-TR												0									1							
1468	1,6-DICHLORO-1,5-CYCLOOCTADIENE												0					0							1				
1469	1,5,8-TRIMETHYL TETRALIN																0			1									
1470	DURENE																0			1	1	1							
1471	TERT-BUTYLBENZENE																		1		1								
1472	4,6-DIMETHYL PYRIMIDINE																		1										
1473	2,3-DIMETHYL PYRAZINE																		1										
1474	PYRAZOLE																		1										
1475	1-METHYL-3-PROPYL BENZENE																			1									
1476	N-PROPYLNAPHTHALENE																			1									
1477	TRIMETHYLNAPHTHALENE																			1		1			1				
1478	TRIMETHYLNAPHTHALENE																			1							0		
1479	TRIMETHYLNAPHTHALENE																			1									
1480	TRIMETHYLNAPHTHALENE																			1									
1481	TRIMETHYLNAPHTHALENE																			1									
1482	TRIMETHYLNAPHTHALENE																			1					1				
1483	TRIMETHYLNAPHTHALENE																			1									
1484	%+ANTHRACENE																			1									
1485	TRIDECANE																			1									

(Continued)

TABLE 11. (Continued)

FINAL REPORT (PART I)

RELATIVE SIZE AND CONCENTRATE WHERE DETECTED

	COMMON NAME	V1C	V1X	T2B	T1C	T1X	T1Y	T4C	T4X	M2C	N2C	P2C	P2X	D2C	D2X	S2C	S2X	L2M	C3C	C1M	C1N	C2N	R1C	R2C	E1C	D2N	B2C	B3C
1486	3-METHYL-3-HEXANOL																		1									
1487	DIETHYLMETHYLVINYLSILANE																		1									
1488	1,3-DISOPROPYL BENZENE																		1									
1489	TETRAHYDROLINALOOL																		1									
1490	2-PHENYL-1,4-CYCLOHEXADIENE																		1									
1491	C3 NAPHTHALENE																		1									
1492	1,4-DIMETHYL-5-OCTYLNAPHTHALENE																		1	1								
1493	ETHYLBENZYL BENZENE (ISOMER UNKNOWN)																		1									
1494	TETRAMETHYL BIPHENYL																		1									
1495	PENTATRIACONTANE																		1									
1496	1,3,5-TRI-TERT-BUTYL BENZENE																		1									
1497	DI-P-TOLYLMETHANE																		1									
1498	DIMETHYLDIPHENYLMETHANE																		1									
1499	X2,3-DIMETHYLNAPHTHALENE																			1								
1500	2-BUTYLNAPHTHALENE																			1								
1501	1,2,4-TRITERTIARY BENZENE																			1								
1502	*P-CHLOROACETOPHENONE																			1								
1503	2,6-DI-TERT-BUTYL TETRALIN																				1							
1504	1,1,3-TRIMETHYL-3-PHENYL INDAN																				1							
1505	1-BROMO-2-CHLOROCYCLOPENTANE																				1							
1506	BETA,BETA-DIMETHYL HISTAMINE																				1							
1507	4-DECANONE																				1							
1508	6-METHYL-2-PHENYLQUINOLINE																					1						
1509	N-BUTYLBENZENE																					1						
1510	HEXAMETHYLENE ACETAMIDE																					1						
1511	4-METHYL-3-HEXANOL																					1						
1512	HEXYL BUTYRATE																					1						
1513	*TRICHLOROBIPHENYL																						1					
1514	2,3,6-TRIMETHYLHEPTANE																						1					
1515	*$HEXACHLOROBIPHENYL																							1				
1516	X*+$DDT																							1				
1517	DIBENZOTHIOPHENE																							1				
1518	4-METHYLDIBENZOTHIOPHENE																							1				
1519	9-ETHYL PHENANTHRENE																							1				
1520	METHYLBENZACRIDINE																							1				
1521	3-ETHYL-5-METHYLPYRIDINE																							1				
1522	N,N-DIETHYLANILINE																							1				
1523	3-DODECANONE																							1				
1524	2,3,4-TRIMETHYLQUINOLINE																							1				
1525	TRIMETHYLQUINONE																							1				
1526	HEXANEDIOIC ACID, DIHEXYL ESTER																							1				
1527	X*P-NITRO PHENOL																								1			
1528	3-CHLORO-2-BUTANOL																								1			
1529	N-CYCLOHEXYLPHENOL																								1		1	
1530	3-METHYLPIPERIDINE-2,6-DIONE																									1		

(Continued)

TABLE 11. (Continued)

FINAL REPORT (PART I)

RELATIVE SIZE AND CONCENTRATE WHERE DETECTED

	COMMON NAME	V1 *C	V1X	T2B	T1C	T1X	T1Y	T4C	T4X	M2C	N2C	P2C	P2X	O2C	O2X	S2C	S2X	L2M	C3C	C1M	C1N	C2N	R1C	R2C	E1C	O2N	B2C	B3C
1531	10-UNDECENOIC ACID																									1		
1532	5-PROPYLDIHYDRO-2-FURANONE																									1		
1533	3A,7A-DIMETHYL OCTAHYDRO-4-ISOBENZOFURAN																									1		
1534	3-METHYL-3-OCTANOL																										1	
1535	BROMODICHLOROANILINE																										1	
1536	6-PHENYL-2-HEXANONE																										1*	
1537	METHYL NONADECANOATE																										1	
1538	HEPTYLPROPIONATE																											1
1539	METHYLCAPRYLIC ACID																											1
1540	ACETAMIDE																											1
1541	DIETHYLENE GLYCOL, MONOMETHYL ETHER																											1
1542	N-BUTYLAMINE																											1
1543	%ETHYL CAPRATE		0											1														
1544	1,3-DIMETHYL-5-(1-METHYLETHYL)-BENZENE							0							1													
1545	2,4-DIMETHYLISOPROPYLBENZENE							1						1														
1546	3-PHENYLPENTANE	a							0*				1*	1														
1547	$N-PROPYL BENZENE											0		1		0												
1548	1,3-DIMETHYL INDAN											0		1														
1549	C6-BENZENE													1														
1550	2-METHYL-2-BUTENAL													1														
1551	3-FUROIC ACID														1													
1552	TETRAHYDRO-3,6-DIMETHYL-2H-PYRAN-2-ONE														1													
1553	2,3-DIMETHYL-1,4-HEXADIENE														1													
1554	2-METHYL-CYCLOHEXANEMETHANOL														1													
1555	3,4-DIHYDRO-1(2H)-NAPHTHALENONE														1													
1556	PENTAMETHYLBENZENE														1													
1557	%ISOQUINOLINE														1													
1558	2,4-DIMETHYLPENTANOL												1															
1559	3,3-DIMETHYLBUTANAMINE												1															
1560	2,7-DIMETHYL TETRALIN	a											1*															
1561	2,4-DIMETHYLHEPTANE												1															
1562	2,6-DIMETHYLHEPTANE												1															
1563	ETHYL BENZOPHENONE	a											1*															
1564	2,4-DICHLOROANILINE							0				1																
1565	%3,4-DICHLOROANILINE							0				1																
1566	2-IODOPENTANE											1																
1567	2-METHYLTHIOPHENE											1																
1568	1,1,3-TRICHLORO-1-BUTENE											1																
1569	1-ETHYL-2,4-DIMETHYL BENZENE											1																
1570	1,6-DIMETHYL-4-ISOPROPYL TETRALIN											1					0											
1571	2-ETHYL-1,3-DIMETHYL BENZENE											1																
1572	2-(METHYLTHIO)BENZOTHIAZOLE											1				0												
1573	NONANAL											1																
1574	INDAN										1					0												
1575	(3-METHYL-2-BUTENYL)BENZENE										1																	

* SEE FOOTNOTE ON LAST PAGE

(Continued)

TABLE 11. (COntinued)

FINAL REPORT (PART I)

RELATIVE SIZE AND CONCENTRATE WHERE DETECTED

	COMMON NAME	V1C	V1X	T2B	T1C	T1X	T1Y	T4C	T4X	M2C	N2C	P2C	P2X	O2C	O2X	S2C	S2X	L2M	C3C	C1M	C1N	C2N	R1C	R2C	E1C	D2N	B2C	B3C
1576	1,4-DIHYDRO-2,5,8-TRIMETHYLNAPHTHALENE										1																	
1577	3,3,3-TRICHLORO-2-METHYLPROPENE									1						-1												
1578	CYCLOHEPTANONE								1																			
1579	BENZYLAMINE								1																			
1580	4,7-DIMETHYL INDAN															0												
1581	BIS(CHLOROPHENYL)METHANE															0												
1582	CIS-4-PHENYLBICYCLOHEXYL															0												
1583	4-METHYLENECYCLOHEXANEMETHANOL															0												
1584	2,6,6-TRIMETHYL-BICYCLO[3.1.1]HEPTAN-3-O															0												
1585	3-BUTYL-1,2,4-CYCLOPENTANETRIONE															0												
1586	%STYRENE GLYCOL															0												
1587	2-METHYL-5-UNDECANONE															0												
1588	(3,3-DIMETHYLCYCLOHEXYLIDENE)ACETALDEHYD															0												
1589	1,2,3,4-TETRAMETHYL BENZENE																0											
1590	1-ETHYL-1-METHYL INDAN																0											
1591	1-CHLOROTETRADECANE																0											
1592	1,1-DIPHENYLCYCLOHEXANE																0											
1593	BICYCLO[2.2.2]OCTANE-1,4-DIOL, MONOACETA																0											
1594	METHYL 3-HYDROXYPHENYLACETATE		0																									
1595	%2-METHYL ANTHRACENE		0																									
1596	2-(PHENYLMETHYL) NAPHTHALENE		0																									
1597	PHENYL P-PYRIDYL KETONE		0																									
1598	DODECYL PHENOL		0																									
1599	FLUOROIODOBENZENE (ISOMER UNKNOWN)																						0					
1600	3-METHYL-2-FURANONE																							0				
1601	2-PHENYL UNDECANE																							0				
1602	1,4,5-TRIMETHYL NAPHTHALENE																							0				
1603	1-TETRADECENE																							0				
1604	DIMETHYL ETHYL BENZENE												0															
1605	1-PHENYL-2-CYCLOPENTEN-1-OL													0														
1606	O-TOLUALDEHYDE													0														
1607	2,3-BIS(METHYLENE)-BICYCLO[3.2.1]OCTANE											0																
1608	2,2-DIMETHYLHEPTANE											0																
1609	1-IODOPENTANE										0																	
1610	%INDENE										0																	
1611	1,2-DIMETHYL INDENE										0																	
1612	1,2-DIHYDRO-1,5,8-TRIMETHYLNAPHTHALENE										0																	
1613	%*+$2-CHLORONAPHTHALENE										0																	
1614	1-ETHYL-3-METHYLCYCLOPENTANE										0																	
1615	DIMETHYL ISOPROPYL BENZENE						0																					
1616	4,6-DIISOPROPYL-M-XYLENE						0																					
1617	7-METHYLBENZOFURAN						0																					
1618	TRICHLOROHEPTAFLUOROBUTANE						0																					
1619	DIMETHYL ISOPROPYL BENZENE						0																					
1620	1,2,3-TRIETHYLBENZENE							0																				

(Continued)

TABLE 11. (Continued)

FINAL REPORT (PART I)

RELATIVE SIZE AND CONCENTRATE WHERE DETECTED

	COMMON NAME	*	V 1 C	V 1 X	T 2 B	T 1 C	T 1 X	T 1 Y	T 4 C	T 4 X	M 2 C	N 2 C	P 2 C	P 2 X	O 2 C	O 2 X	S 2 C	S 2 X	L 2 N	C 3 C	C 1 M	C 1 N	C 2 N	R 1 C	R 2 C	E 1 C	D 2 N	B 2 C	B 3 C
1621	%BENZYL CHLORIDE								-1								-1												
1622	4-METHYLSTYRENE																-1												
1623	2-PHENYLHEXANE																-1												
1624	1,4,6-TRIMETHYL TETRALIN																-1												
1625	4-ISOPROPYL-ALPHA-METHYL STYRENE																-1												
1626	M-TERPHENYL																-1												
1627	DECAHYDRO-1,4A-DIMETHYL-7-(1-METHYLETHYL																-1												
1628	1-CHLORO-4-(1-CHLOROETHENYL)CYCLOHEXENE																-1												
1629	2,4,6-TRIMETHYLBIPHENYL																-1												
1630	4-PHENYLBICYCLOHEXYL																-1												
1631	(1,1#-BICYCLOPENTYL)-2-ONE																-1												
1632	O-TERT-BUTYLPHENOL																-1												
1633	P-(1-ETHYL-1-METHYLHEXYL)PHENOL (A NONY																-1												
1634	P-(2,2,3,3-TETRAMETHYLBUTYL)PHENOL																-1												
1635	ETHYL NONADECANOATE	A																-1											
1636	DIBROMOPHENOL		-1																										
1637	2-(4-METHYL-3-CYCLOHEXENYL)ISOPROPANOL		-1																										
1638	1,2-CYCLOHEXANEDIOL		-1																										
1639	BUTYL THIAZOLE		-1																										
1640	2-HYDROXY-5-ISOPROPYL-2,4,6-CYCLOHEPTATR			-1																									
1641	O-NITROTOLUENE								-1																				

* THE DESIGNATION A AND a DENOTE A COMPOUND THAT IS A PROBABLE OR POSSIBLE ARTIFACT DUE TO XAD-2 RESIN BLEED. RS ENTRIES LABELED WITH AN ASTERISK ARE PROBABLY ATTRIBUTABLE TO THE BLANK ASSOCIATED WITH CONCENTRATE GENERATION. SEE DISCUSSION IN TEXT OF VOLUME 1.

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APPENDIX A
DELIVERABLES

DELIVERABLES REQUIRED BY THE CONTRACT

The deliverables required by EPA Contract 68-03-2548 include the following items:

- monthly progress reports for the first twelve months covering analytical scheme development and validation
- separate reports of analysis results for each analyzed concentrate
- unused portions of concentrates and fractions
- samples of compounds used for identification confirmation
- magnetic tapes of GC-MS data
- utility listings of the databases

Monthly Progress Reports

Monthly progress reports for the first twelve months of contract activity were delivered to the Project Officer on approximately the fifteenth day of the month following the month covered. These reports were dated August 15, 1977 through July 15, 1978.

Concentrate Analysis Reports

Individual reports of concentrate analysis results for DW and AWT concentrates are listed in Tables A1 and A2, respectively. A description of the contents of each of the seven volumes of these reports is given in Table 6, and a description of the material presented in the computer-printed listings is presented in detail in Section V, Analytical Scheme, under "Report Generation/Concentrate Analysis Reports". Three of the concentrates analyzed were process blanks of the concentrate production methodology and are listed in Table A3.

Table A1. Analysis Reports for Drinking Water Concentrates

Code Name[a]	City	Concentrate Type[b]	Date of Report	Concentrates Included in Comb. Rpts.[c]
T1C	Cincinnati, OH	Combined Solvent Extract	08-28-79	
T1X	"	XAD of RO Brine	09-12-79	T1C, T1X
T1Y	"	XAD Direct	10-29-79	T2B[d], T1Y, T1C, T1X
T4C	"	Combined Solvent Extract	04-30-81	
T4X	"	XAD of RO Brine	05-04-81	T4C, T4X
M2C	Miami, FL	Combined Solvent Extract	06-07-79	
M2X	"	XAD of RO Brine	06-26-79	M2C, M2X
N2C	New Orleans, LA	Combined Solvent Extract	07-10-79	
N2X	"	XAD of RO Brine	07-18-79	N2C, N2X
O2C	Ottumwa, IA	Combined Solvent Extract	07-27-79	
O2X	"	XAD of RO Brine	08-03-79	O2C, O2X
P2C	Philadelphia, PA	Combined Solvent Extract	05-21-79	P2C, P2X
P2X	"	XAD of RO Brine	04-20-79	
V1C	Poplarville, MS	Combined Solvent Extract	12-14-79	
V1X	"	XAD of RO Brine	01-07-80	V1C, V1X
S2C	Seattle, WA	Combined Solvent Extract	05-09-79	S2C, S2X
S2X	"	XAD of RO Brine	04-20-79	

a) The code name is used in the computer-printed tables.

b) Combined Solvent Extract: These are extracts of the two RO brines produced. XAD of RO Brine: XAD-2 extraction was performed on the RO brines after solvent extraction.

c) Identified by the three-digit code. Reports with no entry in this column did not contain a combined report.

d) T2B is an XAD-2 resin elution blank, see text.

Table A2. Analysis Reports For Advanced Waste Treatment Water Concentrates

Code Name[a]	City	Concentrate Type[b]	Date of Report	Concentrates Included in Comb. Rpts.[c]
B1M	Blue Plains (Washington D.C.)	$CH_2C\ell_2$ Extract, CA	04-18-20	
B1N	"	Acidic $CH_2C\ell_2$ Extract, CA	11-03-80	B1M and B1N,
B2C	"	Combined Solvent Extract	04-18-80	B1M,B1N & B2C
D2N	Dallas, TX	Acidic $CH_2C\ell_2$ Extract, CA	04-27-81	
E1C	Escondido, CA	Combined Solvent Extract	01-31-80	
R1C	Orange County, CA	Combined Solvent Extract	11-05-79	
R2C	"	Combined Solvent Extract	04-24-81	
C1P	Pomona, CA	Pentane Extract, CA	01-30-79	
C1M	"	$CH_2C\ell_2$ Extract, CA	02-23-79	
C1N	"	Acidic $CH_2C\ell_2$ Extract, CA	04-04-79	C1P,C1M & C1N
C2N	"	Acidic $CH_2C\ell_2$ Extract, CA	04-13-79	C1P,C1M,C1N, C2N & C3C
C3C	"	Combined Solvent Extract	01-15-79	
L2P	Lake Tahoe, CA	Pentane Extract, CA	11-10-78	
L2M	"	$CH_2C\ell_2$ Extract, CA	12-04-78	
L2N	"	Acidic $CH_2C\ell_2$ Extract, CA	12-21-78	L2P,L2M,L2N
L2D	"	Acidic $CH_2C\ell_2$ Extract, Nyl.	04-29-81	L2P,L2M,L2N, and L2D

a) The code name is used in the computer-printed tables.

b) All extracts are of RO brine. "CA" indicate the RO brine produced by the cellulose acetate membrane. "Nylon" refers to RO brine produced by the Permasep R nylon hollow fiber RO unit. "Conbined Solvent Extract" indicates a combination of all extracts of both the CA and Nylon RO brines(a total of six extracts).

c) Identified by the three-digit code. Reports with no entry in this column did not contain a combined report.

Table A3. Analysis Reports for Process for Process Blank Concentrates

Code Name[a]	Sample Description	Date of Report	Concentrates Included in Comb. Rpts.[b]
X1C	evaporated pentane and methylene chloride extraction solvent	11-14-79	
X1X	evaporated ethanol elution solvent of XAD-2 resin	12-05-79	X1C, X1X
T2B[c]	evaporated diethyl ether eluate of XAD-2 resin[c]	08-23-79	T1Y, T2B[c]; T1C, T1X, T1Y, and T2B

a) The code name is used in the computer-printed tables.

b) Identified by the three-digit code. Reports with no entry in this column did not contain a combined report.

c) Concentrate T2B is a process blank for concentrate T1Y only (see table A1)

Unused Portions of Concentrates

Unused portions of DW and AWT concentrates were stored at -10°C at Battelle until the GC-MS analysis tasks were completed. These unused concentrate portions were hand-delivered to the Project Officer in May, 1980. The returned aliquots, except as explained below, consisted of 10 percent and 40 percent of the material originally produced for the solvent extracted and XAD-2 extracted concentrates, respectively.

Generally, the portion received by Battelle of concentrates produced by solvent extraction of RO brine was 20 percent of the total produced from the sampled water. Half of the material submitted (10 percent) was partitioned into fractions for GC-MS analysis. The remaining material (10 percent of the total produced) was used for sample archiving and analysis of the concentrate, as received; these GC-MS and residue weight analyses consumed only about 1.5 percent of the 10 percent saved. If it became necessary to repeat the fractionation of the concentrate, the entire remaining amount was used, and this occurred for six concentrates: V1C and V1X (Table 1A), C1N (Table 2A), and X1C, X1X and T2B (Table 3A).

Generally, concentrates produced by XAD-2 resin extraction of RO brine were supplied for analysis in the amount of 50 percent of the total material. Use of 10 percent for GC-MS analysis thus left 40 percent of the originally produced material for sample archiving and repeated analysis, if necessary. Repeated analyses of concentrates P2X, S2X and O2X (Table 1A) reduced the unused portions to 30, 20 and 30 percent of the originally produced material, respectively.

Three of the AWT concentrates (B2C, E1C and R2C, Table 2A) were incorrectly divided into aliquots for biological (toxicity) testing and GC-MS analysis before being sent by EPA to Battelle. The aliquot received was 16 percent (20 percent of 80 percent) of the original material produced. Partitioning of 10 percent thus left 6 percent remaining for unpartitioned concentrate analysis and sample archiving. Fortunately, repeat analysis was not required for these three samples.

Unused Portions of Fractions

As explained under Section V, Analytical Scheme/Residue Weight Analysis, a variable amount, ranging from 10 to 60 percent, of each concentrate fraction and corresponding blank was consumed for the determination of residue weights. The remainder of each sample was sealed into a 2.0 ml break-seal glass ampule for sample archiving and stored at -10°C. These ampules were delivered to the Project Officer along with the unused portions of the concentrates.

Aliquots of Reference Standards

Compound identifications were confirmed by GC-MS analysis of commercially obtained standards whenever possible and practical. GC-MS data for 1035 different compounds were obtained for this purpose. An aliquot of each of these compounds except for those supplied as mixtures was placed in a 1.8 ml

Teflon-sealed screw cap bottle and delivered to the Project Officer.

Magnetic Tapes of GC-MS Data

The GC-MS data acquired during the course of the Contract can be classified as follows:

- GC-MS analysis of unpartitioned concentrates, fractions and corresponding blanks
- GC-MS analysis of confirmation standards and standard mixtures of the compounds for specific search
- MS calibration verification and DFTPP ion source tuning verification data corresponding to each GC-MS data file described above
- SGCSM GC-MS performance verification for each day that the above described data were obtained

All of the above data were stored on 9-track magnetic tape. When repeat analyses were required, the unused, previously acquired data were not deleted from the tape archive, so that the collection of 89 tapes actually corresponds to all acquired data. The tapes were numbered sequentially and each tape is accompanied by a computer-printed listing which shows the data files on the tape (by the 6-digit data system file name) and the amount of storage space required for it on a magnetic disk in system/150 "block" storage units. The 6-digit data file naming system used for the analysis of unpartitioned concentrates, fractions and corresponding method blanks was designed to eliminate the possibility of using the same file name for more than one sample analysis. In addition, the file name readily translates into a complete description of the sample using the directions included in each concentrate report and reproduced with some expansion in Appendix B. The 6-digit code naming system unambiguously identifies the following:

- the city, the sampling sequence number, and the method of organic extraction from RO brine
- identity of the fraction (or unpartitioned concentrate)
- the GC phase used for the analysis
- indication as the first, second, etc., time that the analysis had been performed
- for the mass calibration, DFTPP and SGCSM performance verifications, the 6-digit name identifies the type of GC-MS quality assurance check and the data file to which the QA check file corresponds.

Utility Listings of the Databases

Computerized data management of both the compound identification results and the chromatographic data from analysis of reference standards allowed the listing of these databases in multiple orderings that were valuable beyond their relevance to the contract work. These two sets of listings were produced in a one-volume format (for each database) and multiple copies delivered to the Project Officer. The contents of these two special supplementary reports and a description of the information provided in the listings is given in Section V, Analytical Scheme in this volume of the Final Report (see Special Listings of the Database and Compound Identification and Confirmation). Note that the report volume covering the confirmation standards database also serves as a source guide for EPA users of the GC-MS standards repository which was created from the set of aliquots of reference compounds delivered to the Project Officer (described above in this Appendix under Aliquots of Reference Standards). The repository is managed by the Environmental Monitoring Support Laboratory (EMSL) at EPA-Cincinnati, and the computer-printed listing of the confirmation database is available from Dr. Bill Budde at EMSL-CI.

ADDITIONAL DELIVERABLES PROVIDED BY BATTELLE

System/150 Data Processing and Utility Programs

In order to make GC-MS data acquisition and processing on the Systems Industries System/150 GC-MS data system more effective and efficient, development of some new software was required. In addition, the existing data acquisition program (IFSS) was modified to allow the use of a real-time internal clock for accurate assignment of GC retentions. Two of the new programs written for this work can be classified as relatively complex data processing capability providing extracted ion current profile (EICP) data searching and graphics. The remaining eight are relatively simple data handling programs. All of these programs, listed and described below, were delivered to the Project Officer on a magnetic disk for distribution to other EPA GC-MS laboratories.

Data Processing Programs

1. Selected Ion Summation (SIS)—The SIS program provided new and more powerful EICP processing and convenient, flexible chromatography graphics display/output capabilities. Some of the capabilities include:

- display of the summed ion current of one to eight ions with the absence in a given spectrum of any one of the selected ions resulting in the sum for that spectrum to be set to zero

- variable thresholding requiring the least intense of the selected ions to be a user-selected percent of the most intense

- base peak requirement option which sets the EICP sum to zero unless the user-designated base peak is the largest of the selected ions

- chromatographic display of up to 2047 spectra on one page of the CRT screen or plotter output with the summed EICP trace synchronized with (and appearing above) the total ion chromatogram trace

- easy GC peak area determination, chromatographic scale expansion, and retention time determination using the CRT terminal cross-hairs; independent vertical scale expansion of EICP and total ion traces

- automatic queue forming of spectrum-background pairs using the CRT terminal cross-hairs

- selection of local or global normalization of the total ion chromatogram trace

2. Selected Ion Summation Data Search for Specified Compounds (QSIS)--The QSIS program allowed automated searching of GC-MS data for any number of species. The parameters for the individual compounds (output labeling, retention time, selected EICP ions, etc.) are established by a separate program (see EDQ, below). The signal level thresholding and EICP zero-set defaulting described above for the SIS program are incorporated for the EICP data search. Other features of the QSIS program include:

- searching of a user-specified width GC retention window based on either relative or absolute retention

- option to pause after searching for each compound for spectrum-background queuing or area determination, as described for the SIS program. There is no pause if no EICP peaks are detected

- automatic plotting on one 8 1/2 by 11 inch page of the SIS EICP trace and the total ion trace (vertically correlated) over the selected GC retention window. No plot is produced if no EICP peaks are detected

Utility Data Handling Programs

1. Search Queue Editor (EDQ)--The EDQ program was required to set up a file of compounds for automated data searching using the QSIS software described above. For each search compound entry in the list, the following are specified: name of the compound; the SIS ions (one to eight); ion thresholding to be used; base peak requirement, if any; and expected retention time and/or relative retention index. The program allows editing by deletion or modification of the entries which are accessed by their sequence numbers. New entries can also be added to the end of the list, and there is no practical limit to the number of compounds that can be placed in such a search queue.

2. Magnetic Tape Storage/Retrieval (MAG150)--The MAG150 program allowed GC-MS data files to be transfered to and retrived from standard 9-track magnetic tape using the System/150 data system. Data are stored on tape in an industry-standard (800 bits/inch) format using a data file specific dialogue

rather than the entire disk image as the storage unit. The software is designed for use with a Digital Equipment Corp. TM-8E-compatible interface and a Wangco Model 10 tape handling unit. Nine to eleven GC-MS data files and their associated performance verification checks can be stored on a single 2400 ft. tape.

3. Spectrum Queue Handling Programs (MERGE, QSORT and BUILDQ)--These three programs aided in manipulating lists (queues) of spectrum-background pairs (Q-files) in preparation for library matching and spectrum plotting. MERGE allows two or more Q-files to be combined into a new Q-file with a new, user-specified name. The QSORT program can then be used to sort the spectrum-background pairs of a Q-file by increasing order of the spectrum number. The BUILDQ program allows Q-files to be listed on the CRT terminal or printer showing the number of entries and the spectrum/background numbers in the list. This program also allows new Q-files to be created by typing in the spectrum/background pairs at the CRT terminal.

4. Data Interpretation Worksheet (QFORM)--The QFORM program created a tabular format for recording mass spectral-based compound identification results. For each entry of a referenced Q-file, the form shows a sequence number, the spectrum number, the subtracted background spectrum number, the retention time, the relative retention index, and designated spaces to record the compound identity, molecular weight, molecular formula, size of the GC peak, library match index and confidence level of the analyst. Each page of the form is labeled with the data file name and the retention time of the internal standard and a space is provided for the name of the analyst and the date of completion. The form is printed on standard 15-inch wide z-fold computer form paper with 26 entries per page.

5. Data Transfer from System/150 to INCOS (QSAVE and INCOS4)--Since the Finnigan INCOS mass spectral library matching software was distinctly superior to that available on the System/150 data system, two new programs were required to accomplish the transfer of mass spectral data between the two systems. The QSAVE program constructs a user-named data file of the background subtracted mass spectra corresponding to the entries of a Q-file of interest. This greatly abbreviated data file (usually 75 to 300 spectra compared to the 2100 to 2800 spectra of the original data file) can then be transfered directly to the INCOS data system using the INCOS4 software. Spectrum library matching can be performed on each spectrum of this abbreviated data file using standard INCOS software. The hard-copied output of the INCOS library match is correlated to the original data via the sequence number of the abbreviated data file and the sequence number on the Data Interpretation Worksheet produced by the QFORM program (see No. 4, above). The INCOS4 program can also be used to transfer full (unabbreviated) GC-MS data files. Retention time information is not retained in the transfered data file.

MASS SPECTRAL LIBRARY IMPLEMENTATION

When the 31,357 EPA/NIH/NSRDS mass spectral library became available from the National Bureau of Standards, it was immediately implemented at Battelle's GC-MS facility for the INCOS data system. This implementation was done one year before the expanded library was made available through the instrument manufacturer (Finnigan Instruments). The 31,357 spectrum library was supplied to the Project Officer on a standard INCOS data system magnetic disk for distribution to interested EPA GC-MS facilities.

Preliminary Report on DW Concentrate Analyses for Five Cities

At the conclusion of analyses of the first ten DW concentrates a preliminary combined report of the compound identification results and residue weight analysis results was prepared at the request of the Project Officer. These ten concentrates were the five pairs of combined solvent extracts and XAD-2 extracts of the RO brine produced from the second sampling of five cities: Miami, Florida; Philadelphia, Pennsylvania; New Orleans, Louisiana; Ottumwa, Iowa; and Seattle, Washington.

This report contained the following items:

- summary of the special interest compounds found among the total of 1152 identified compounds
- brief explanation of the analytical scheme
- discussion of the compound identification and residue weight analysis results and assessment of the problem of artifact compounds due to XAD-2 resin bleed
- three listings of the 1152 identified compounds in the format described in this Final Report volume under Section V, Analytical Scheme Report Generation/Combined Concentrate Analysis Reports.

This combined report was classified as preliminary due to the following three circumstances: 1. Analysis of the five Cincinnati DW concentrates had not been completed and, thus, were not included. 2. Assessment of the RO method blanks (the two Poplarville, Mississippi DW concentrates) had not been completed. 3. Further compound identification confirmation for the results of these five cities was anticipated. The Final Report material in this volume and Volume 2 completes these three requirements, and, thus, supercedes the preliminary report on the five cities.

Fifty bound copies of the preliminary five cities DW report were delivered on August 28, 1979 to the Project Officer. This report is available through U.S. EPA HERL/CI.

APPENDIX B

SYSTEM FOR NAMING GC-MS DATA FILES

The Systems Industries System/150 GC-MS data system which was used for all GC-MS data acquisition in this work allowed a maximum of six digits to be used for naming GC-MS data files. A naming system was developed which both eliminated the possibility of replicate use of a data file name and allowed relatively easy translation of the six digits, in a logical and systematic fashion, to a completely unambiguous description of the sample.

Only three digits of this 6-digit code (the second, third and fourth) are used in the Final Report material covering the DW and AWT concentrates. These three digits code the city, sampling sequence and method of concentrate production and, thus, completely identify the concentrate. Four digits (the second, third, fourth and fifth) were required to code the twenty small-volume samples associated with the Cincinnati DW GAC Contactor A and D samplings. Since these 3- or 4-digit sample identifying codes are always translated in the accompanying text and/or tables, knowledge of the complete 6-digit coding system, as presented in this appendix, is not necessary for understanding any part of the Final Report. Access of the original GC-MS data on 9-track tape (one of the deliverables listed in Appendix A) does, however, require the use of the 6-digit file name coding system. For this reason, the following complete explanation has been included here.

Digit One

A number was used to identify the fraction analyzed as follows:

0 = Unprocessed concentrate, as received
1 = Base fraction
2 = Acid fraction (derivatized)
3 = 2.75 ml hexane eluate from silica gel
4 = Neutral compounds (no acids or bases); no other fractionation
5 = 4 ml hexane/benzene eluate from silica gel
6 = 4 ml methylene chloride eluate from silica gel
7 = 4 ml methanol eluate from silica gel
8 = Combination of 1, the base fraction, and 6, the CH_2Cl_2 eluate
9 = 4 ml methylene chloride eluate of silica gel following the 2.75 ml hexane elution (i.e., hexane/benzene elution omitted)

Digit Two

A letter was used to indicate the origin of the water sample as follows:

B = Blue Plains, Washington, D. C.(AWT)
C = Pomona, California (AWT)
D = Dallas, Texas (AWT)
E = Escondido, California (AWT)
J = Jefferson Parrish (New Orleans) Louisiana (DW)
L = Lake Tahoe, California (AWT)
M = Miamia, Florida (DW)
N = New Orleans, Louisiana (DW)
O = Ottumwa, Iowa (DW)
P = Philadelphia, PA (DW)
R = Orange County, CA (AWT)
S = Seattle, WA (DW)
T = Cincinnati, Ohio (DW)

V = Poplarville, MS (DW)
X = An extraction solvent blank

Digit Three

Numbers 1 to 6 were used to indicate the sampling sequence of the site.

Digit Four

For large-volume concentrates, a letter corresponding to the method of extraction of organic material from the RO brine was used:

C = Combination of all RO brine solvent extracts
D = Acidified methylene chloride extraction of RO brine from the nylon membrane
P = Pentane extraction of RO brine from the cellulose acetate membrane
M = Methylene chloride extraction of RO brine from the cellulose acetate membrane
N = Acidified methylene chloride extraction of RO brine from the cellulose acetate membrane
X = XAD extraction of RO brine with ethanol elution
Y = Direct XAD extraction of the sampled water with diethyl ether elution; RO processing was not used
B = A blank elution of an XAD column using diethyl ether

For small-volume water samples, letters were used to indicate the point of sampling for all samples except the Jefferson Parrish XAD/analytical samples:

Q = A "Super-Q" reagent water 10-liter extraction blank
L = 10 liters of water, lyophylized and reconstituted to the original volume with "Super-Q" reagent water
K = 10 liters of water corresponding to L, above
E = 10 liters of water sampled prior to RO concentration and GAC contactor treatment
R = Water sampled from various points in the RO concentration process at a volume approximating 10 liters of unconcentrated water
G = Water following GAC contactor treatment, unconcentrated or concentrated 200-fold by RO
Y = A concentrate produced by XAD-2 extraction/diethyl ether elution

XAD analytical samples generated from reverse osmosis concentration process monitoring of the Jefferson Parrish sampling are coded with a number as follows:

Sampling Point of the RO Concentrator	pH of Sample Before XAD-2 Extraction	
	Acidic	Basic
Cellulose Acetate Feed	1	2
Cellulose Acetate Permeate (Nylon Feed)	3	4
Cellulose Acetate Concentrate	5	6
Nylon Concentrate	7	8

The number 9 in the third digit indicates the sample is a blank XAD elution.

Digit Five

For the large-volume DW and AWT concentrates and all small-volume samples except those corresponding to the Cincinnati GAC contactors A and D, the following letter/number system was used to indicate whether the data file corresponded to an analysis on the SP1000 or SP2100 GC column as well as to indicate the type of GC-MS performance verification, where applicable:

1 = Sample analyzed using the SP1000 GC column
A = FC43 by batch inlet to check mass calibration corresponding to a sample analysis using SP1000
B = Direct inlet check of DFTPP prior to sample run using SP1000 column
C = GC-MS analysis of the SGCSM system test mixture prior to sample analysis using SP1000 column

2 = Sample analyzed using the SP2100 GC column
D = FC43 by batch inlet to check mass calibration corresponding to a sample analysis using SP2100
E = Direct inlet check of DFTPP prior to sample run using SP2100 column
F = GC-MS analysis of the SGCSM system test mixture prior to analysis run using SP2100 column

For the twenty small-volume samples corresponding to Cincinnati GAC contactors A and D, a letter/number combination was used for the fourth/fifth digits to completely identify the point of sampling. The only GC column used for all the small-volume samples was SP1000, so this parameter did not need identification in the fifth digit of the 6-digit code. The second and third digits for the 13 GAC Contactor A and 7 GAC Contactor D samples are T4 and T5, corresponding to the fourth and fifth Cincinnati sampling, respectively. The following is the coding system for the fourth and fifth digits for these twenty samples:

T4 Samples[a]		T5 Samples[b]	
Digits 4 and 5	Sample Identity[c]	Digits 3 and 4	Sample Identity[c]
E1	10 liters, finished DW	E1	10 liters, finished DW
R1	10-fold, CA conc.	R1	10-fold, CA conc.
R2	100-fold, CA conc.	R2	10-fold, NYL conc.
R3	10 liters, CA permeate	R3	200-fold, CA conc.
R4	10-fold, NYL conc.	R4	200-fold, CA conc.
R5	100-fold, NYL conc.	G1	10 liters
R6	200-fold, CA conc.	Y1	XAD-2 concentrate
G1	10 liters		
G2	200-fold, CA conc.		
Y1	10 liters, XAD-2 permeate, Na_2SO_3 preserved		
Y2	XAD-2 concentrate corresponding to Y1		
Y3	10 liters, XAD-2 permeate, without Na_2SO_3		
Y4	XAD-2 concentrate corresponding to Y3		

a) Only G1 and G2 are post-GAC samples.
b) Only E1 and R4 are pre-GAC samples.
c) 10-fold, etc. indicates the degree of RO concentration; CA conc. and NYL conc. are RO concentrates from cellulose acetate and nylon membranes, respectively.

Indication of the GC-MS performance verification data for these twenty small-volume samples was accomplished somewhat differently than as described above for the large-volume samples:

Performance Check	Correspondence of Letters with the Numbers Used to Identify the Twenty Small-Volume Samples					
	1	2	3	4	5	6
FC-43	A	D	G	J	M	P
DFTPP	B	E	H	K	N	Q
SGCSM	C	F	I	L	O	R

Digit Six

A number was used corresponding to whether the data file resulted from the first, second, etc., time analysis was attempted; or, if the sample corresponded to a blank, a letter was used. Thus, "A" would indicate the first attempt to analyze a blank sample, "B" the second attempt, and so on.

EXAMPLE TRANSLATIONS

The following examples illustrate the use of the above mechanism for translating 6-digit GC-MS file names into sample identities:

2L2D2B: The second analysis of the process blank (-----B) on the SP2100 GC column (----2-) of the derivatized acid fraction (2-----) corresponding to the derivatized acid fraction of the AWT concentrate produced from the second sampling (--2---) at Lake Tahoe (-L----) by methylene chloride extraction of the acidified RO brine produced with the nylon membrane (---D--).

5P2X11: The first analysis (-----1) of the hexane/benzene silica gel eluent (5-----) of the DW concentrate produced from the second sampling (--2---) at Philadelphia (-P----) by XAD-2 extraction of RO brine (---X--) analyzed on the SP1000 GC column (----1-).

7T4CEA: A DFTPP GC-MS performance check (----E-) corresponding to the first analysis (using SP2100 GC column (----E-)) of the process blank (-----A) methanol elution of silica gel (7-----) generated with the fractionation of the DW concentrate of the fourth sampling (--4---) at Cincinnati (-T----) which was a composite of all the solvent extracts of RO brine (---C--).

APPENDIX C

PUBLICATIONS AND PRESENTATIONS RESULTING FROM THE CONTRACT WORK

At this writing, five reports containing results of the contracted research have been published in the scientific literature:

1. Lin, D.C.K., R.G. Melton, F.C. Kopfler, and S.V. Lucas, "Chapter 46. Glass Capillary GC-MS Analysis of Organic Concentrates from Drinking and Advanced Waste Treatment Water", p. 861, in Advances in the Identification and Analysis of Organic Pollutants in Water, Vol. 2, L.H. Keith, Ed., Ann Arbor Science Publishers, 1981

2. Melton, R.G., W.E. Coleman, R.W. Slater, F.C. Kopfler, W.K. Allen, T.A. Aurand, D.E. Mitchell, S.J. Voto, S.C. Watson, and S.V. Lucas, "Chapter 36. Comparison of Grob Closed-Loop-Stripping Analysis (CLSA) to Other Trace Organic Methods", p. 597, in Advances in the Identification and Analysis of Organic Pollutants in Water, Vol. 2, L.H. Keith, Ed., Ann Arbor Science Publishers, 1981.

3. Lin, D.C.K., S.V. Lucas, B.A. Petersen, R.G. Melton, and W.E. Coleman, "Glass Capillary GC-MS Analysis of Organics in Drinking Water Concentrates and Advanced Waste Treatment Water Concentrates", in High Resolution Gas Chromatography, S.P. Cram, Ed., Academic Press, New York.

4. Lin, D.C.K., R.L. Foltz, S.V. Lucas, B.A. Petersen, and L.E. Slivon, "Application of Deuterated Standards in Analysis of Organics in Water Concentrates", in Stable Isotopes: Proceedings from Third International Conference, p. 243, R. Klein and P. Klein, Eds., Academic Press, New York (1979)

5. Lin, D.C.K., R.L. Foltz, S.V. Lucas, B.A. Petersen, L.E. Slivon, and R.G. Melton, "Glass Capillary GC-MS Analysis of Organics in Drinking Water Concentrates and Advanced Waste Treatment Water Concentrates. II.", in Measurement of Organic Pollutants in Water and Wastewater, p. 68, E.E. Van Hall, Ed., ASTM Special Technical Publication, No. 686, Philadelphia, Pennsylvania (1979).

Publications 1 and 2 were presented in lectures given by Lucas and Melton, respectively at the Symposium on Analysis of Organic Pollutants in Water at the American Chemical Society meeting, August, 1980 in Las Vegas, Nevada. Publications 4 and 5 were presented in a talk by Lin at the Third International Conference on Stable Isotopes in 1978 at Argonne National Laboratory and the ASTM Committee D-19 meeting in June, 1978, at Denver, Colorado, respectively. The following oral presentations at scientific meetings do not have corresponding written publications. In each case the first author listed made the oral presentation:

1. Petersen, B.A., R.L. Foltz, S.V. Lucas, and D.C.K. Lin, "Routine Evaluation and Optimization of a Capillary Column GC/Quadrupole MS/COM System for the Analysis of Complex Environmental Samples", Twenty-Sixth Annual Conference on Mass Spectrometry and Allied Topics, St. Louis, May 31, 1978.

2. Slivon, L.E., "A Selected Ion Summation Technique Used for Reverse Search and Quantitation", Twenty-sixth Annual Conference on Mass Spectrometry and Allied Topics, St. Louis, May 31, 1978.

3. Contos, D.A., V.R. Goff, S.V. Lucas, S.C. Watson, L.E. Slivon, and D.C.K. Lin, "Glass Capillary GC-MS Analysis of Organic Pollutants in Water. I. Fractionation and Analysis of Complex Concentrates from Drinking Water and Advanced Waste Treatment Water," 11th Central Regional Meeting, American Chemical Society, Columbus, Ohio, May 7, 1979.

4. Goff, V.R., D.A. Contos, S.V. Lucas, S.C. Watson, L.E. Slivon, and D.C.K. Lin, "Organic Pollutants in Water. II. Quality Assurance, Results, and Computerized Data Searching for Specific Pollutants in the Analysis of Complex Concentrates from Drinking Water and Advanced Waste Treatment Water", 11th Central Regional Meeting, American Chemical Society, Columbus, Ohio, May 7, 1979.

5. Lin, D.C.K., R.L. Foltz, S.V. Lucas, and B.A. Petersen, "Glass Capillary GC-MS Analysis of Drinking and Advanced Waste Treatment Water Concentrates". Presented at the Twenty-seventh Annual Conference on Mass Spectrometry and Allied Topics, June 4, 1979, Seattle, Washington.

6. Lucas, S.V., B.A. Petersen, R.L. Foltz, and D.C.K. Lin, "Routine Performance Monitoring of a Capillary GC/Quadrupole MS/Computer System Used for the Analysis of Complex Environmental Pollution Samples". Presented at the Twenty-seventh Annual Conference on Mass Spectrometry and Allied Topics, June 4, 1979, Seattle, Washington.

In addition, two publications in refereed journals (probably Environmental Science and Technology and the Journal of the American Water Works Association) are planned.

APPENDIX D

IDENTIFIED COMPOUNDS LISTED BY MOLECULAR WEIGHT

Tables of computer-printed listings of identified compounds accompany the discussion of the DW and AWT results in this volume. Analogous tables for the small-volume samples are presented in Volume 3 of this Final Report. All of these tables list the identified compounds in decreasing order of the size of the observed GC peak while showing in which of the concentrates identification occurred. Thus, these tables provide for a convenient comparison of occurrence in related concentrates as well as an easy visualization of the predominant chemical species present. However, since these lists are ordered by decreasing size of the GC peak, it is difficult to determine if and where a specific compound was found. Obviously, the ability to determine whether a specific compound was found in these concentrates is of critical importance to the present and future usefulness of this work. To accomplish compound-specific inspection of the results, Table D1 has been produced. This table lists all the compounds that have been added to the computer-managed database by increasing molecular weight, and correlates this listing with the tables showing occurrence of the compounds in the four sets of related samples (DW, AWT, GAC contactor A and GAC contactor D). Thus, to determine whether a specific compound was found, the range of compounds in Table D1 which have the correct molecular weight must be searched. If the compound is found in Table D1, it can then be located at the indicated sequence number of the relevant table showing the concentrates or small-volume samples in which that compound was found. Tables 9 and 10 of this Final Report volume are correlated in Table D1 for the DW and AWT concentrates, respectively, and Tables 7 and 8 of Volume 3 are correlated for the GAC contactor A and D samples, respectively.

For a few of the compounds in Table D1, detection in any of the four groups of samples is not indicated. A brief description of the structure and use of the identified compound database provides an explanation for this apparent inconsistency. The database of identified compounds is structured on two levels. The first level contains information about chemical species; i.e., name, CAS registry number, molecular weight, molecular formula, types of functional groups, industrial source and use, etc., but contains no concentrate-specific information. The second level contains exclusively (except for the CAS registry number) concentrate-specific information; i.e., the concentrate and fraction where identified, size of the GC peak, identification proof status, retention time, relative retention index, and spectrum number, and it is linked to the first level of the database only by the CAS registry number. The listing in Table D1 is of the first, chemically descriptive level of the database. There are three principal reasons that some entries in Table D1 are not listed further in the four sample-specific occurrence tables:

- The compounds identified in the set of nine Jefferson Parrish small-volume samples were entered in the database but are not included in the set of four sample groups. These nine samples were so grossly contaminated with XAD-2 resin bleed artifacts that many of the identified species were not found even in other samples which had substantial XAD-2 resin bleed contamination and are included in the DW sample group. There are 91 compounds in Table 1D which were not found in the four data sets and can unambiguously be attributed to this source. These materials are typically aromatic hydrocarbons, some of which contain oxygen.

- Some compounds were deliberately added to the database for convience in anticipation of their detection in samples but were not subsequently detected in the four sample groups. Isomers of commonly encountered species or high interest compounds such as the 53 specific search compounds are included in this category. Twenty of the specific search entries in Table D1 were not found in any sample.

- Preliminary compound identification results were sometimes added to the first, chemically descriptive level of the database before final review by a senior analyst. In these cases, compound identifications that were disallowed were, of course, not entered into the second, concentrate-specific level of the database. However, these compounds were not removed from the first level (since the possibility always existed to correctly identify the compound in subsequent analyses), so they still appear in Table D1.

Of the 2107 entries in Table D1, 271 are not reported as having been found in one of the four groups of samples with which the table is correlated.

TABLE D1. COMPOUNDS IN THE CHEMICALLY DESCRIPTIVE LEVEL OF THE IDENTIFIED COMPOUND DATA BASE--LISTED BY INCREASING MOLECULAR WEIGHT

IDENTIFIED COMPOUNDS BY MOLECULAR WEIGHT
NOTE--THIS LIST MAY CONTAIN COMPOUNDS THAT HAVE NOT BEEN FOUND IN ANY OF THE CONCENTRATES ANALYZED

MW	CAS NO.	COMMON NAME	DATA SET CORRELATION † DW	AMT	T4	T5	MOLECULAR FORMULA
55	624793	ISOCYANOETHANE	921				C3 . H5 . N1
55	38239279	N-METHYL ETHENAMINE	662				C3 . H5 . N1
59	60355	ACETAMIDE		1079			C2 . H5 . N1 . O1
60	71238	XPROPYL ALCOHOL	104		158		C3 . H8 . O1
60	64197	ACETIC ACID	580				C2 . H4 . O2
62	107211	XETHYLENE GLYCOL	960	832			C2 . H6 . O2
62	75014	VINYL CHLORIDE	1037				C2 . H3 .CL1
62	455	CARBONIC ACID					C1 . H2 . O3
68	288131	PYRAZOLE		902			C3 . H4 . N2
68	142290	CYCLOPENTENE	650				C5 . H8
72	598323	3-BUTEN-2-OL	985				C4 . H8 . O1
73	68122	XDMF (DIMETHYL FORMAMIDE)	1070	314			C3 . H7 . N1 . O1
73	109739	N-BUTYLAMINE		1087			C4 . H11. N1
74	71363	X1-BUTANOL	5	22	117		C4 . H10. O1
74	75650	XTERT-BUTANOL	586				C4 . H10. O1
74	78922	SEC-BUTYL ALCOHOL	734				C4 . H10. O1
74	109944	ETHYL FORMATE					C3 . H6 . O2
75	107142	CHLOROACETONITRILE	564				C2 . H2 . N2 .CL2
76	109864	ETHYLENE GLYCOL, MONOMETHYL ETHER	533	623	33	86	C3 . H8 . O2
76	109875	XMETHYLAL	602	896			C3 . H8 . N2
76	3031752	ISOPROPYL HYDROPEROXIDE	262				C3 . H8 . O2
79	584032	1,2-BUTANEDIOL				87	C4 . H10. O2
79	110861	X*PYRIDINE	573	460			C5 . H5 . N1
80	107073	2-CHLOROETHANOL					C2 . H5 . O1 .CL1
82	110838	XCYCLOHEXENE		254			C6 . H10
82	917920	3,3-DIMETHYLBUTYNE	1128				C6 . H10
82	534225	2-METHYLFURAN	851	746			C5 . H6 . O1
82	930303	2-CYCLOPENTEN-1-ONE	89				C5 . H6 . O1
84	75092	XMETHYLENE CHLORIDE					C1 . H2 .CL2
84	625332	3-PENTEN-2-ONE	65	946			C5 . H8 . O1
84	34314835	2,3-DIHYDRO-4-METHYLFURAN	183				C5 . H8 . O1
84	497030	TIGALDEHYDE	830				C5 . H8 . O1
84	120923	CYCLOPENTANONE	538				C5 . H8 . O1
84	765435	XCYCLOPROPYL METHYL KETONE	175				C5 . H8 . O1
84	1115113	2-METHYL-2-BUTENAL					C5 . H8 . O1
85	616455	2-PYRROLIDONE			18		C4 . H7 . N1 . O1
86	108054	VINYL ACETATE		569			C4 . H6 . O2
86	107879	XMETHYL PROPYL KETONE		99			C5 . H10. O1
86	4675870	2-METHYL-2-BUTEN-1-OL	279				C5 . H10. O1
86	556821	3-METHYL-2-BUTEN-1-OL	80	947			C5 . H10. O1
86	625310	4-PENTEN-2-OL	922	897			C5 . H10. O1
86	4401110	1-OXIRANYLETHANONE	620				C4 . H6 . O2
86	5076197	TRIMETHYLOXIRANE	831				C5 . H10. O1
86	115184	2-METHYL-3-BUTEN-2-OL	114				C5 . H10. O1
86	1569501	3-PENTEN-2-OL	55	497			C5 . H10. O1

† SEE FOOTNOTE ON LAST PAGE

(Continued)

TABLE D1. (Continued)

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IDENTIFIED COMPOUNDS BY MOLECULAR WEIGHT
NOTE--THIS LIST MAY CONTAIN COMPOUNDS THAT HAVE NOT BEEN FOUND IN ANY OF THE CONCENTRATES ANALYZED

MW	CAS NO.	COMMON NAME	DATA SET CORRELATION †				MOLECULAR FORMULA
			DW	AWT	T4	T5	
86	1003141	PROPYLOXIRANE	293				C5 . H10. O1
86	431038	%DIACETYL					C4 . H6 . O2
86	3724650	%CROTONIC ACID	1038				C4 . H6 . O2
86	96480	%BUTROLACTONE	426				C4 . H6 . O2
86	96220	DIETHYL KETONE		593			C5 . H10. O1
88	141786	%ETHYL ACETATE		210		162	C4 . H8 . O2
88	126998	%*CHLOROPRENE					C4 . H5 .CL1
88	123911	%1,4-DIOXANE	266	171	114		C4 . H8 . O2
88	79312	%ISOBUTYRIC ACID	113	418			C4 . H8 . O2
88	107926	%BUTYRIC ACID	24	389			C4 . H8 . O2
88	6032297	1-METHYLBUTYLALCOHOL	54	684			C5 . H12. O2
88	584021	DIETHYL CARBINOL	181	745			C5 . H12. O2
88	71410	%N-AMYL ALCOHOL	683	895			C5 . H12. O1
88	598754	SEC-ISOAMYL ALCOHOL	1129	1003			C5 . H12. O1
88	107891	ALDOL	121				C4 . H8 . O2
88	513860	ACETOIN	1113				C4 . H8 . O2
88	75854	%TERT-PENTYL ALCOHOL	530				C5 . H12. O1
88	75843	NEOPENTYL ALCOHOL		703			C5 . H12. O1
88	96311	N,N'-DIMETHYLUREA	402				C3 . H8 . N2 . O1
88	554121	METHYL PROPIONATE					C4 . H8 . O2
88	625547	ETHYL ISOPROPYL ETHER			43		C5 . H12. O1
89	51796	%URETHANE (ETHYLCARBAMATE)	951				C3 . H7 . N1 . O2
90	563473	%3-CHLORO-2-METHYL PROPENE	142	506			C4 . H7 .CL1
90	107982	1-METHOXY-2-PROPANOL	45	103			C4 . H10. O2
90	107880	1,3-BUTYLENE GLYCOL		629			C4 . H10. O2
90	110805	%ETHYLENE GLYCOL MONOETHYL ETHER((OXITOL(CELLOSOLVE)	567	717			C4 . H10. O2
90	144627	%OXALIC ACID	1040				C2 . H2 . O4
90	1589475	2-METHOXY-1-PROPANOL		318	115		C4 . H10. O2
90	513859	2,3-BUTANEDIOL		481			C4 . H10. O2
90	50215	2-HYDROXYPROPANOIC ACID					C3 . H6 . O3
92	108883	%$TOLUENE	62	324	250		C7 . H8
92	1340337	*1-CHLORO-2,3-EPOXYPROPANE ((CHLOROMETHYL)OXIRANE)					C3 . H50. O1 .CL1
92	78955	%CHLOROACETONE	729	712			C3 . H50. O1 .CL1
93	108996	B-PICOLINE		554			C6 . H7 . N1
93	62533	%*ANILINE	582				C6 . H7 . N1
93	109068	ALPHA-PICOLINE	842	657			C6 . H7 . N1
93	108894	GAMMA-PICOLINE	961				C6 . H7 . N1
94	108952	%*+PHENOL	156	208	163		C6 . H6 . O1
94	67710	DIMETHYLSULFONE	925	387			C2 . H6 . O2 . S1
94	79118	%CHLOROACETIC ACID	724	1080	228		C2 . H3 . O2 .CL1
94	127004	1-CHLORO-2-PROPANOL			160		C3 . H7 . O1 .CL1
94	74839	BROMOMETHANE			132		C1 . H3 .BR1
96	591480	3-METHYLCYCLOHEXENE		505			C7 . H12
96	930687	2-CYCLOHEXENONE	139	369			C6 . H8 . O1
95	108974	4H-PYRAN-4-ONE		864			C5 . H4 . O2

† SEE FOOTNOTE ON LAST PAGE

(Continued)

TABLE D1. (Continued)

WATER POLLUTANTS PAGE 3

IDENTIFIED COMPOUNDS BY MOLECULAR WEIGHT

NOTE--THIS LIST MAY CONTAIN COMPOUNDS THAT HAVE NOT BEEN FOUND IN ANY OF THE CONCENTRATES ANALYZED

MW	CAS NO.	COMMON NAME	DATA SET CORRELATION † DW	AWT	T4	T5	MOLECULAR FORMULA
96	1120736	2-METHYL-2-CYCLOPENTEN-1-ONE	864			131	C6 . H8 . O1
96	2758181	3-METHYL-2-CYCLOPENTEN-1-ONE	590		150	135	C6 . H8 . O1
96	4562270	X4(1H)-PYRIMIDINONE	322				C4 . H4 . N2 . O1
96	10111087	1H-IMIDAZOLE-2-CARBOXALDEHYDE	92	1103			C4 . H4 . N2 . O1
96	20521420	2-VINYLCROTONALDEHYDE	552				C6 . H8 . O1
96	98011	%FURFURAL	1025			195	C5 . H4 . O2
98	107062	X$1,2-DICHLOROETHANE	332	306			C2 . H4 .CL2
98	1120725	2-METHYLCYCLOPENTANONE	711	498			C6 . H10. O1
98	1757422	3-METHYLCYCLOPENTANONE	154	179			C6 . H10. O1
98	108941	%CYCLOHEXANONE	16	568			C6 . H10. O1
98	141797	XMESITYL OXIDE (3-ISOHEXEN-2-ONE)		233		70	C6 . H10. O1
98	822673	2-CYCLOHEXENOL		830			C6 . H10. O1
98	291645	SUBERANE					C7 . H14
98	505577	2-HEXENAL		668			C6 . H10. O1
98	109499	ALLYLACETONE	1153				C6 . H10. O1
98	758872	3-METHYL-4-PENTEN-2-ONE	545				C6 . H10. O1
98	49607514	1-METHYL-1H-1,2,4-TRIAZOL-3-AMINE					C3 . H6 . N4
98	625650	2,4-DIMETHYL-2-PENTENE	605				C7 . H14
98	554143	2-METHYLTHIOPHENE					C5 . H6 . S1
98	5362505	4-METHYL-3-PENTENAL	482				C6 . H10. O1
98	25044013	2-METHYL-1-PENTEN-3-ONE	789				C6 . H10. O1
98	16015115	3,4-DIHYDRO-6-METHYL-2H-PYRAN	550				C6 . H10. O1
98	2497214	4-HEXEN-3-ONE	43				C6 . H10. O1
98	592778	2-HEPTENE	27				C7 . H14
98	286204	X7-OXABICYCLO[4.1.0]HEPTANE	572		103	38	C6 . H10. O1
98	25659227	4-HEXEN-2-ONE		470			C6 . H10. N1
98	108872	HEXAHYDROTOLUENE	66				C7 . H14
98	2008	PHOSPHORIC ACID					H3 . O4 . P1
98	111284	2,4-HEXADIEN-1-OL	180	181			C6 . H10. O1
98	456	PHOSPHORIC ACID					H3 . O4 . P1
99	22122367	3-METHYL-2-FURANONE		1099			C5 . H6 . O2
99	872504	%N-METHYL-2-PYROLIDONE	543	487	95		C5 . H9 . N1 . O1
99	1768247	BUTYL CYANATE	916				C5 . H9 . N1 . O1
99	27154434	PIPERIDINONE	437	459			C5 . H9 . N1 . O1
99	2141620	3-ETHOXYPROPIONITRILE	979				C5 . H9 . N1 . O1
100	25144052	CIS-2-METHYLCYCLOPENTANOL	94	361			C6 . H12. O1
100	591786	XMETHYL BUTYLKETONE	177	65			C6 . H12. O1
100	589388	HEXAN-3-ONE	720	150	40		C6 . H12. O1
100	2088075	2-METHYL-1-PENTEN-3-OL	269	800			C6 . H12. O1
100	108101	XMETHYL ISOBUTYL KETONE		215			C6 . H12. O1
100	108930	%CYCLOHEXANOL	10	309			C6 . H12. O1
100	2144414	CIS-2,5-DIMETHYLTETRAHYDROFURAN		420			C6 . H12. O1
100	53778613	2,3,4-TRIMETHYLOXETANE		849			C6 . H12. O1
100	1003389	2,5-DIMETHYL THF		850			C6 . H12. O1
100	142825	HEPTANE					C7 . H16

† SEE FOOTNOTE ON LAST PAGE

(Continued)

TABLE D1. (Continued)

IDENTIFIED COMPOUNDS BY MOLECULAR WEIGHT
NOTE--THIS LIST MAY CONTAIN COMPOUNDS THAT HAVE NOT BEEN FOUND IN ANY OF THE CONCENTRATES ANALYZED

MW	CAS NO.	COMMON NAME	DATA SET CORRELATION † DW	AWT	T4	T5	MOLECULAR FORMULA
100	24070777	2-METHYLCYCLOPENTANOL (GEOMETRY UNKNOWN)	176	446			C6 . H12. O1
100	25144041	TRANS-2-METHYLCYCLOPENTANOL	21	879			C6 . H12. O1
100	3586581	2-METHYLENEBUTYRIC ACID	566	922			C5 . H8 . O2
100	541479	3-METHYL-2-BUTENOIC ACID	99				C5 . H8 . O2
100	626982	2-PENTENOIC ACID	1016				C5 . H8 . O2
100	542289	TETRAHYDRO-2H-PYRAN-2-ONE	876				C5 . H8 . O2
100	111342	X1-(ETHENYLOXY)BUTANE	122				C6 . H12. O1
100	1192229	3-ETHYL-2,2-DIMETHYLOXIRANE	836				C6 . H12. O1
100	108292	DIHYDRO-5-METHYL-2(3H)-FURANONE	329	728			C5 . H8 . O2
100	15877573	3-METHYLPENTANAL	229	706			C6 . H12. O1
100	53778624	2-ETHYL-3-METHYLOXETANE	493				C6 . H12. O1
100	16173383	2-ETHYL-1,3,2-DIOXABOROLANE	495				C4 . H9 . O2 . B1
100	54774275	5-HEXEN-2-OL	682	727			C6 . H12. O1
100	6124909	CIS-2,3-EPOXYHEXANE	833				C6 . H12. O1
100	5076200	TETRAMETHYLOXIRANE					C6 . H12. O1
100	15045600	1,3-EPOXY-4-METHYLPENTANE					C6 . H12. O1
100	565695	2-METHYL-3-PENTANONE	1086				C6 . H12. O1
100	5204648	3-PENTENOIC ACID	1039				C5 . H8 . O2
100	17257793	METHYL PROPENYLOXY KETONE	957				C5 . H8 . O2
100	97961	2-ETHYLBUTANAL	57	86			C6 . H12. O1
101	617845	N,N-DIETHYL FORMAMIDE	270	555	147	113	C5 . H11. N1 . O1
101	3850304	3,3-DIMETHYLBUTANAMINE					C6 . H15. N1
101	541468	ISOVALERAMIDE	969	607			C5 . H11. N1 . O1
101	5329793	2-HEXANEAMINE	179	180			C6 . H15. N1
101	6859990	PIPERIDINOL		302			C5 . H11. N1 . O1
102	1120974	4-METHYL DIOXANE		330			C5 . H10. O2
102	111273	1-HEXANOL	679	943	183		C6 . H14. O1
102	77747	3-METHYLPENTAN-3-OL	201	491			C6 . H14. O1
102	623370	3-HEXANOL	46	214	25		C6 . H14. O1
102	626937	2-HEXANOL	193	178			C6 . H14. O1
102	116530	2-METHYLBUTYRIC ACID	22	202			C5 . H10. O2
102	109524	%VALERIC ACID	95	204	159		C5 . H10. O2
102	503742	ISOVALERIC ACID	63	106			C5 . H10. O2
102	108112	4-METHYL-2-PENTANOL	35	177	127	83	C6 . H14. O1
102	55185	%*DIETHYLNITROSAMINE					C4 . H10. N2 . O1
102	1185337	2,2-DIMETHYL-1-BUTANOL		277			C6 . H14. O1
102	541504	ACETOACETIC ACID	1011	442			C4 . H6 . O3
102	115220	3-HYDROXY-3-METHYL-2-BUTANONE	630	1054			C5 . H10. O2
102	97994	TETRAHYDROFURFURYL ALCOHOL; THFA	931				C5 . H10. O2
102	75989	PIVALIC ACID	254				C5 . H10. O2
102	594605	2,3-DIMETHYL-2-BUTANOL	147				C6 . H14. O1
102	2866851	3-ETHOXYPROPANAL	888				C5 . H10. O2
102	590363	2-METHYL-2-PENTANOL	362				C6 . H14. O1
102	592847	BUTYL FORMATE	777				C5 . H10. O2
102	36839675	3-METHOXYPENTANE	100			98	C6 . H14. O1

† SEE FOOTNOTE ON LAST PAGE

(Continued)

TABLE D1. (Continued)

WATER POLLUTANTS PAGE 5

IDENTIFIED COMPOUNDS BY MOLECULAR WEIGHT

NOTE--THIS LIST MAY CONTAIN COMPOUNDS THAT HAVE NOT BEEN FOUND IN ANY OF THE CONCENTRATES ANALYZED

MW	CAS NO.	COMMON NAME	DATA SET CORRELATION † DW	AWT	T4	T5	MOLECULAR FORMULA
102	36960222	1-HYDROXY-3-METHYL-2-BUTANONE	832				C5 . H10. O2
102	3393644	4-HYDROXY-3-METHYL-2-BUTANONE	837				C5 . H10. O2
102	4016119	%(ETHOXYMETHYL)OXIRANE	295				C5 . H10. O2
102	96402	3-CHLOROCYCLOPENTENE	255				C5 . H7 .CL1
102	108214	ISOPROPYL ACETATE	730				C5 . H10. O2
102	7326467	TETRAHYDRO-2-METHYL-2-FURANOL	438	146			C5 . H10. O2
102	2679870	2-ETHOXYBUTANE					C6 . H14. O1
102	589355	3-METHYL-1-PENTANOL	994				C6 . H14. O1
103	100470	BENZONITRILE	377	845	138	77	C7 . H5 . N1
104	100425	%*$STYRENE	130	334			C8 . H8
104	141822	%MALONIC ACID		611			C3 . H4 . O4
104	53778737	1-METHOXY-2-BUTANOL		443			C15. H12. O2
104	17773658	2-CHLORO-3-METHYL-2-BUTENE	881				C5 . H9 .CL1
104	111320	4-METHOXY-1-BUTANOL	610				C5 . H12. O2
104	683705	3-CHLORO-3-BUTEN-2-ONE	923				C4 . H5 . O1 .CL1
104	594616	2-HYDROXY-2-METHYLPROPANOIC ACID	6				C4 . H8 . O3
104	5166358	3-CHLORO-2-METHYL-1-BUTENE	823				C5 . H9 .CL1
104	7778850	1,2-PROPYLENE GLYCOL, DIMETHYL ETHER	26				C5 . H12. O2
104	694871	BICYCLO(4.2.0)OCTA-1,3,5-TRIENE					C8 . H8
104	2807309	N-PROPOXY ETHANOL	710				C5 . H12. O2
104	4744109	1-1-DIMETHOXYPROPANE	162				C5 . H12. O2
104	10471144	1-ETHOXY-1-METHOXYETHANE	161				C5 . H12. O2
104	13417431	1-CHLORO-2-METHYL-2-BUTENE	348				C5 . H9 .CL1
104	53778720	3-METHOXY-2-BUTANOL		295			C5 . H12. O2
104	5694688	1,3-DIOXALANE METHANOL				190	C4 . H8 . O3
104	3587642	1-METHOXY-2-METHYL-2-PROPANOL					C5 . H12. O2
106	95476	%$O-XYLENE	776	750	167	84	C8 . H10
106	108383	%$M-XYLENE	141	511	41	46	C8 . H10
106	106423	%$P-XYLENE	417	173	166	82	C8 . H10
106	100414	$ETHYLBENZENE	416	172	42	81	C8 . H10
106	100527	%BENZALDEHYDE	115	160	30		C7 . H6 . O1
106	628900	METHYL METHOXYMETHYL FORMAL		617			C4 . H10. O3
106	598798	2-CHLORO-2-PROPENOIC ACID	927				C3 . H3 . O2 .CL1
106	543599	AMYL CHLORIDE	106				C5 . H11.CL1
106	753899	NEOPENTYL CHLORIDE	349				C5 . H11.CL1
106	111466	DIETHYLENE GLYCOL			108		C4 . H10. O3
106	539800	2,4,6-CYCLOHEPTATRIEN-1-ONE					C7 . H6 . O1
107	108485	%2,6-LUTIDINE	694	618			C7 . H9 . N1
107	108474	%2,4-LUTIDINE	695	1055			C7 . H9 . N1
107	536754	4-ETHYLPYRIDINE	1079				C7 . H9 . N1
107	583619	2,3-LUTIDENE	696	886			C7 . H9 . N1
107	589935	2,5-LUTIDINE	962	1056			C7 . H9 . N1
107	8894	BENZYLAMINE					C7 . H9 . N1
108	1558174	4,6-DIMETHYL PYRIMIDINE		980			C6 . H8 . N2
108	5910894	2,3-DIMETHYL PYRAZINE		981			C6 . H8 . N2

† SEE FOOTNOTE ON LAST PAGE

(Continued)

TABLE D1. (Continued)

IDENTIFIED COMPOUNDS BY MOLECULAR WEIGHT
NOTE--THIS LIST MAY CONTAIN COMPOUNDS THAT HAVE NOT BEEN FOUND IN ANY OF THE CONCENTRATES ANALYZED

MW	CAS NO.	COMMON NAME	DATA SET CORRELATION † DW	AWT	T4	T5	MOLECULAR FORMULA
108	108394	%META-CRESOL		297	229	185	C7 . H8 . O1
108	106445	%*P-CRESOL		308	170	183	C7 . H8 . O1
108	95487	%O-CRESOL	199	348			C7 . H8 . O1
108	100516	%BENZYL ALCOHOL	182	268	100		C7 . H8 . O1
108	1603414	2-AMINO-5-PICOLINE		846			C6 . H8 . N2
108	598787	ALPHA-CHLOROPROPIONIC ACID	821				C3 . H5 . O2 .CL1
108	111693	DICYANOHEXANE	90				C6 . H8 . N2
108	100663	METHOXYBENZENE					C7 . H8 . O1
108	563848	3-CHLORO-2-BUTANOL		1070			C4 . H9 . O1 .CL1
109	3018120	DICHLOROACETONITRILE				132	C2 . H1 . N1 .CL2
110	1193186	3-METHYL-2-CYCLOHEXEN-1-ONE	450	383			C7 . H10. O1
110	280331	BICYCLO[2.2.2] OCTANE					C8 . H14
110	1192627	%2-ACETYLFURAN	596	658			C6 . H6 . O2
110	53783872	2-NORBORNENE-7-OL		667			C7 . H10. O1
110	34167759	3-PROPYLCYCLOPENTENE	462			137	C8 . H14
110	1674108	1,2-DIMETHYLCYCLOHEXENE	608				C8 . H14
110	14072867	4,4-DIMETHYLCYCLOHEXENE	893				C8 . H14
110	53783883	3-METHOXY-1,3,4-HEXATRIENE	281				C7 . H10. O1
110	931884	CYCLOOCTENE					C8 . H14
110	5771324	SPIRO(2.4)HEPTAN-2-ONE					C7 . H10. O1
110	620020	5-METHYLFURFURAL	1014				C6 . H6 . O2
110	18669528	2,3-DIMETHYL-1,4-HEXADIENE					C8 . H14
111	629083	N-HEXYLCYANIDE					C7 . H13. N1
111	6407358	N-CYCLOHEXYLIDENE METHANAMINE					C7 . H13. N1
112	16106595	4,5-DIMETHYL-1-HEXENE		378			C8 . H16
112	20019641	5,5-DIMETHYL-2-FURANONE	251	585	151	115	C6 . H8 . O2
112	111660	1-OCTENE		401			C8 . H16
112	108907	%CHLOROBENZENE	640	432		71	C6 . H5 .CL1
112	88142	%2-FUROIC ACID	1151				C5 . H4 . O3
112	34314846	2,3-DIHYDRO-4-(1-METHYLETHYL)FURAN	318				C7 . H12. O1
112	5166530	5-METHYL-3-HEXEN-2-ONE	874				C7 . H12. O1
112	2511913	PENTYL TRIMETHYLENE					C8 . H16
112	7740694	3-ETHOXY-3-METHYL-1-BUTYNE	491				C7 . H12. O1
112	6004600	1-CYCLOPENTYLETHANONE	400	304			C7 . H12. O1
112	80717	2-HYDROXY-3-METHYL-2-CYCLOPENTEN-1-ONE	30				C6 . H8 . O2
112	3726474	1-ETHYL-3-METHYLCYCLOPENTANE					C8 . H16
112	23758272	1-METHYL-2-CYCLOHEXEN-1-OL	1077				C7 . H12. O1
112	33061164	1-METHYL-3-CYCLOHEXEN-1-OL	108				C7 . H12. O1
112	1713333	1-METHYL-7-OXABICYCLO[4.1.0]HEPTANE					C7 . H12. O1
112	110441	%SORBIC ACID					C6 . H8 . O2
112	488937	3-FUROIC ACID					C5 . H4 . O3
112	16747505	1-ETHYL-METHYLCYCLOPENTANE					C8 . H16
112	123331	%1,2-DIHYDRO-3,6-PYRIDAZINEDIONE	574	687			C4 . H4 . N2 . O2
112	684946	3,4-DIMETHYL-3-PENTEN-2-ONE		939			C7 . H12. O1
112	6714007	5-HEPTEN-2-ONE		937			C7 . H12. O1

† SEE FOOTNOTE ON LAST PAGE

(Continued)

TABLE D1. (Continued)

WATER POLLUTANTS PAGE 7

IDENTIFIED COMPOUNDS BY MOLECULAR WEIGHT
NOTE--THIS LIST MAY CONTAIN COMPOUNDS THAT HAVE NOT BEEN FOUND IN ANY OF THE CONCENTRATES ANALYZED

MW	CAS NO.	COMMON NAME	DATA SET CORRELATION †				MOLECULAR FORMULA
			DW	AWT	T4	T5	
112	502421	CYCLOHEPTANONE				130	C7 . H12. O1
113	1121922	OCTAHYDROAZOCINE		859			C7 . H15. N1
113	931204	N-METHYL-2-PIPERIDINONE		938			C6 . H11. N1 . O1
113	105602	HEXAHYDRO-2H-AZEPINE-2-ONE		608			C6 . H11. N1 . O1
114	589435	2,4-DIMETHYL HEXANE					C8 . H18
114	123193	4-HEPTANONE	296	328	67		C7 . H14. O1
114	110134	2,5-HEXANEDIONE	202	378	93	64	C6 . H10. O2
114	3123975	5,5-DIMETHYLDIHYDROFURANONE	244	129			C6 . H10. O2
114	5145017	3,5-DIMETHYLDIHYDROFURANONE		130			C6 . H10. O2
114	110430	METHYL N-AMYL KETONE	386	261		85	C7 . H14. O1
114	695067	5-ETHYLDIHYDRO-2(3H)-FURANONE	1059	598			C6 . H10. O2
114	592278	2-METHYLHEPTANE					C8 . H18
114	56052950	TRANS-2-ETHYL-3-PROPYLOXIRANE		847			C7 . H14. O1
114	823223	6-METHYL-TETRAHYDRO-2-PYRANONE		436			C6 . H10. O2
114	14925963	2-BUTYL-3-METHYLOXIRANE	284	596			C7 . H14. O1
114	17257817	3,4-EPOXY-2-HEXANONE	264	323			C6 . H10. O2
114	56052836	1-METHOXY-2-HEXENE		440			C7 . H14. O1
114	41065978	4-METHYLHEXANAL		867	9		C7 . H14. O1
114	502443	%6-HYDROXYCAPROIC ACID LACTONE		447			C6 . H10. O2
114	106354	ETHYL BUTYL KETONE	819	876			C7 . H14. O1
114	41653934	TRANS-3-METHYL-3-PENTENOIC ACID	1058				C6 . H10. O2
114	1191044	2-HEXENOIC ACID	385	592			C6 . H10. O2
114	1577226	5-HEXENOIC ACID	1126				C6 . H10. O2
114	623563	ETHYL ISOBUTYL KETONE	601				C7 . H14. O1
114	4478631	1-(3,3-DIMETHYLOXIRANYL)ETHANONE	798				C6 . H10. O2
114	3521913	1-HEPTEN-4-OL	268				C7 . H14. O1
114	7493585	ACETYL ISOBUTYRYL	606				C6 . H10. O2
114	592132	2,5-DIMETHYLHEXANE					C8 . H18
114	17257828	3,4-EPOXY-3-ETHYL-2-BUTANONE	611				C6 . H10. O2
114	17612350	2,2-DIMETHYL-3-PROPYLOXIRANE	898				C7 . H14. O1
114	53897328	2-ETHYL-3-PROPYLOXIRANE	1136				C7 . H14. O1
114	5363633	1-(ETHNYLOXY)PENTANE	909				C7 . H14. O1
114	27944792	2,4-DIMETHYLPENTANAL	834				C7 . H14. O1
114	931566	METHOXYCYCLOHEXANE	1110				C7 . H14. O1
114	13861977	4,4-DIMETHYLDIHYDROFURANONE	200	317			C6 . H10. O2
114	53229393	(1-METHYLBUTYL)OXIRANE	553	499			C7 . H14. O1
114	53897317	2-METHYL-2-ISOBUTYLOXIRANE	282				C7 . H14. O1
114	533608	2-HYDROXYCYCLOHEXANONE	554				C6 . H10. O2
114	33467764	2-HEPTENOL	560	738			C7 . H14. O1
114	1860395	5-METHYLHEXANOL	531				C7 . H14. O1
114	123206	VINYL BUTYRATE	539				C6 . H10. O2
114	53229417	3-METHYLBUTYLOXIRANE					C7 . H12. O1
114	42328438	2-METHYL-2-(1-METHYLPROPYL)-OXIRANE	1027				C7 . H14. O1
114	4528261	ALLYL-1,3-DIOXANE	371				C6 . H10. O2
114	598398	2,2-DICHLOROETHANOL					C2 . H4 . O1 .BR1

† SEE FOOTNOTE ON LAST PAGE

(Continued)

TABLE D1. (Continued)

IDENTIFIED COMPOUNDS BY MOLECULAR WEIGHT

NOTE--THIS LIST MAY CONTAIN COMPOUNDS THAT HAVE NOT BEEN FOUND IN ANY OF THE CONCENTRATES ANALYZED

MW	CAS NO.	COMMON NAME	DATA SET CORRELATION † DW	AWT	T4	T5	MOLECULAR FORMULA
114	110123	METHYL ISOPENTYL KETONE		594			C7 . H14. O1
114	7379126	2-METHYL-3-HEXANONE				97	C7 . H14. O1
114	598389	2,2-DICHLOROETHANOL			105		C2 . H4 . O1 .CL2
114	1436357	2-T-BUTYL-3-ETHYLOXIRANE					C8 . H16. O1
116	1070833	3,3-DIMETHYLBUTYRIC ACID	547	32			C6 . H12. O2
116	142621	%CAPROIC ACID	155	71	21	68	C6 . H12. O2
116	7319235	HEX-3-ENE-2,5-DIOL		796			C6 . H12. O2
116	88095	2-ETHYLBUTYRIC ACID	800	203			C6 . H12. O2
116	595379	2,2-DIMETHYL BUTYRIC ACID	799	102			C6 . H12. O2
116	97610	2-METHYL VALERIC ACID	475	563			C6 . H12. O2
116	123422	DIACETONE ALCOHOL	419	325			C6 . H12. O2
116	123864	N-BUTYL ACETATE		219			C6 . H12. O2
116	105431	3-METHYL VALERIC ACID	453	205			C6 . H12. O2
116	646071	ISO-HEXANOIC ACID	224	377			C6 . H12. O2
116	14287617	2,3-DIMETHYLBUTYRIC ACID	517	379			C6 . H12. O2
116	95136	%INDENE		992			C9 . H8
116	597966	3-METHYL-3-HEXANOL		999			C7 . H16. O1
116	18641811	SEC-BUTYLISOPROPYL ETHER	536	641			C7 . H16. O1
116	123762	LEVULINIC ACID	267	645	213	102	C5 . H8 . O3
116	632224	%TETRAMETHYLUREA, TMU		650			C5 . H12. N2 . O1
116	2313657	3-METHYL-2-HEXANOL	603	1018			C7 . H16. O1
116	100721	TETRAHYDROPYRAN-2-METHANOL		662			C6 . H12. O2
116	3970625	2,2-DIMETHYL-3-PENTANOL	380	670			C7 . H16. O1
116	595415	2,3-DIMETHYL-3-PENTANOL		444			C7 . H16. O1
116	615292	4-METHYL-3-HEXANOL		1032			C7 . H16. O1
116	589559	DIPROPYL CARBINOL	1154	877			C7 . H16. O1
116	111706	HEPTYL ALCOHOL	389	878	148		C7 . H16. O1
116	543497	METHYL AMYL CARBINOL	306	327			C7 . H16. O1
116	617298	2-METHYL-3-HEXANOL	56	87			C7 . H16. O1
116	589822	3-HEPTANOL	347	452	240		C7 . H16. O1
116	623552	5-METHYL-3-HEXANOL	278				C7 . H16. O1
116	600362	2,4-DIMETHYLPENTANOL					C7 . H16. O1
116	627598	5-METHYL-2-HEXANOL	772	471			C7 . H16. O1
116	766972	4-METHYLSTYRENE					C9 . H8
116	36687986	3-METHOXY-3-METHYL-2-BUTANONE	42	1101	118	45	C6 . H12. O2
116	54774286	TETRAHYDRO-5-METHYL-2-FURANMETHANOL	540				C6 . H12. O2
116	625230	2-METHYL-2-HEXANOL	906				C7 . H16. O1
116	822833	2-ISOPROPYL-1,3-DIOXOLANE	619				C6 . H12. O2
116	17429048	5-METHOXY-2-PENTANONE	1142				C6 . H12. O2
116	2370129	2,2-DIMETHYL-1-PENTANOL	231				C7 . H16. O1
116	625069	2,4-DIMETHYL-2-PENTANOL	783				C7 . H16. O1
116	4911700	2,3-DIMETHYL-2-PENTANOL	822				C7 . H16. O1
116	627985	5-METHYL-1-HEXANOL	555	714			C7 . H16. O1
116	53102140	3-CHLORO-2-CYCLOPENTEN-1-ONE	557				C5 . H5 . O1 .CL1
116	766154	4,4-DIMETHYL-1,3-DIOXANE	801				C6 . H12. O2

† SEE FOOTNOTE ON LAST PAGE

(Continued)

TABLE D1. (Continued)

IDENTIFIED COMPOUNDS BY MOLECULAR WEIGHT
NOTE--THIS LIST MAY CONTAIN COMPOUNDS THAT HAVE NOT BEEN FOUND IN ANY OF THE CONCENTRATES ANALYZED

MW	CAS NO.	COMMON NAME	DATA SET CORRELATION † DW	AWT	T4	T5	MOLECULAR FORMULA
116	759057	3-METHYL-2-OXO-BUTANOIC ACID					C5 . H8 . O3
116	61142776	2,3-DIMETHYLTETRAHYDRO-2-FURANOL		453			C6 . H12. O2
116	123442	4-HYDROXY-4-METHYL-2-PENTANONE	117	479			C6 . H12. O2
116	931179	1,2-CYCLOHEXANEDIOL		1105			C6 . H12. O2
116	4359450	2-ETHYL-4-METHYL-1,3-DIOXOLANE				39	C6 . H12. O2
116	2441976	3-CHLOROCYCLOHEXENE			140		C6 . H9 .CL1
116	34632896	1-CHLORO-2,4-HEXADIENE				40	C6 . H9 .CL1
116	930654	4-CHLOROCYCLOHEXENE				129	C6 . H9 .CL1
117	140294	%BENZYL CYANIDE	346	458	130	79	C8 . H7 . N1
117	7175475	1-ISOCYANO-4-METHYLBENZENE	151				C8 . H7 . N1
118	496117	INDAN		771			C9 . H10
118	105577	ACETALDEHYDE DIETHYL ACETAL		509			C6 . H14. O2
118	67663	%CHLOROFORM					C1 . H1 .CL3
118	111762	2-BUTOXYETHANOL	210	148			C6 . H14. O2
118	611154	*2-METHYL STYRENE		802			C9 . H10
118	637503	1-ALLYLBENZENE	1053	1000		50	C9 . H10
118	4799626	PENTAMETHYLENE GLYCOL, MONOMETHYL ETHER		630			C6 . H14. O2
118	271896	COUMARONE		861			C8 . H6 . O1
118	2935446	2,5-HEXANEDIOL	681	153			C6 . H14. O2
118	629118	1,6-HEXANEDIOL	317	666			C6 . H14. O1
118	542187	CYCLOHEXYL CHLORIDE	755				C6 . H11.CL1
118	97643	ETHYL LACTATE	119				C5 . H10. O3
118	105588	%ETHYL CARBONATE	307	929			C5 . H10. O3
118	76095	PINACOL	1144				C6 . H14. O2
118	98839	ISOPROPENYLBENZENE	485				C9 . H10
118	29006028	4-METHOXYBUTANOIC ACID					C5 . H10. O3
118	3739308	2-HYDROXY-2-METHYLBUTANOIC ACID					C5 . H10. O3
118	4026180	2-HYDROXYISOVALERIC ACID					C5 . H10. O3
118	18243215	TRIMETHYLSILYL FORMATE					C4 . H10. O2
118	110156	%SUCCINIC ACID	439				C4 . H6 . O4
118	1569013	1-PROPOXY-2-PROPANOL		913			C6 . H14. O2
118	107415	2-METHYL-2,4-PENTANEDIOL		147			C6 . H14. O2
118	1779197	1,3,6-TRIOXOCANE		465			C5 . H10. O3
118	873494	CYCLOPROPYLBENZENE				89	C9 . H10
120	611143	O-ETHYL TOLUENE	1076	333			C9 . H12
120	98828	%$CUMENE		523	187	23	C9 . H12
120	526738	1,2,3-TRIMETHYL BENZENE	797	513	223		C9 . H12
120	620144	1-ETHYL-3-METHYL BENZENE	795	545	215	7	C9 . H12
120	108678	%MESITYLENE	806	514	216		C9 . H12
120	103651	$N-PROPYL BENZENE		951			C9 . H12
120	95636	PSEUDOCUMENE	1010	337	168		C9 . H12
120	98862	%ACETOPHENONE	67	559	141	19	C8 . H8 . O1
120	622968	P-ETHYL TOLUENE	1112	769		25	C9 . H12
120	623698	1,3-DIMETHOXY-2-PROPANOL	618	430			C5 . H12. O3
120	16197903	4-CHLOROCROTONIC ACID	858	1081			C4 . H5 . O2 .CL1

† SEE FOOTNOTE ON LAST PAGE

(Continued)

TABLE D1. (continued)

IDENTIFIED COMPOUNDS BY MOLECULAR WEIGHT
NOTE--THIS LIST MAY CONTAIN COMPOUNDS THAT HAVE NOT BEEN FOUND IN ANY OF THE CONCENTRATES ANALYZED

MW	CAS NO.	COMMON NAME	DATA SET CORRELATION † DW	AWT	T4	T5	MOLECULAR FORMULA
120	40529031	4-CHLORO-3-BUTENOIC ACID					C4 . H5 . O2 .CL1
120	529204	O-TOLUALDEHYDE					C8 . H8 . O1
120	126330	TETRAHYDRO-1,1-DIOXIDE THIOPHENE		154		147	C4 . H8 . O2 . S1
120	111773	DIETHYLENE GLYCOL, MONOMETHYL ETHER		1086	179	187	C5 . H12. O3
121	108758	2,4,6-COLLIDINE	697	844			C8 . H11. N1
121	622322	BENZALDEHYDEOXIME					C7 . H7 . N1 . O1
121	1122390	2,4,5-COLLIDINE	966	1057			C8 . H11. N1
121	695987	2,3,5-COLLIDINE	1170	1059			C8 . H11. N1
121	104905	5-ETHYL-2-PICOLINE	964				C8 . H11. N1
121	1462846	2,3,6-TRIMETHYLPYRIDINE	963	1061			C8 . H11. N1
121	2233296	2,3,4-TRIMETHYLPYRIDINE	965				C8 . H11. N1
121	1122696	2-ETHYL-6-PICOLINE	967				C8 . H11. N1
121	3999788	3-ETHYL-5-METHYLPYRIDINE		1060			C8 . H11. N1
122	65850	%BENZOIC ACID	17	10	2	1	C7 . H6 . O2
122	105679	%+*2,4-DIMETHYLPHENOL (XYLENOL)		591			C8 . H10. O1
122	95807	%*2,4-DIAMINOTOLUENE					C7 . H10. N2
122	104938	P-METHYLANISOLE		848			C8 . H10. O1
122	90006	PHLOROL	1061				C8 . H10. O1
122	98851	%METHYLPHENYL CARBINOL		303			C8 . H10. O1
122	100834	3-HYDROXYBENZALDEHYDE	839				C7 . H6 . O2
122	123079	4-ETHYLPHENOL		730			C8 . H10. O1
122	95658	3,4-DIMETHYLPHENOL				186	C8 . H10. O1
122	108689	3,5-DIMETHYLPHENOL					C8 . H10. O1
123	98953	%*+$NITROBENZENE	652		79	151	C6 . H5 . N1 . O2
124	1123097	3,5-DIMETHYL-2-CYCLOHEXEN-1-ONE	988	596			C8 . H12. O1
124	90051	%GUAIACOL	1155	869			C7 . H8 . O2
124	496106	OCTAHYDROINDENE	774				C9 . H16
124	24156954	3,5,5-TRIMETHYL-2-CYCLOPENTEN-1-ONE	773	597			C8 . H12. O1
124	23799259	1-METHYL-4-METHYLENESUBERANE	604				C9 . H16
124	25172069	3,7-OCTADIEN-2-ONE	559				C8 . H12. O1
124	55683211	3,4,5-TRIMETHYL-2-CYCLOPENTEN-1-ONE	959	1085			C8 . H12. O1
124	28790865	2,3,4-TRIMETHYL-2-CYCLOPENTEN-1-ONE	1013	935			C8 . H12. O1
124	150765	%P-METHOXYPHENOL (HYDROQUINONE, MONOMETHYL ETHER)					C7 . H8 . O2
124	932661	1-(1-CYCLOHEXEN-1-YL)ETHANONE	1050				C8 . H12. O1
124	1484541	6-METHYL-BICYCLO[4.1.0]HEPTANONE	1024				C8 . H12. O1
124	16647044	6-METHYL-3,5-HEPTADIEN-2-ONE	1026	925			C8 . H12. O1
124	504154	%ORCINOL	752				C7 . H8 . O2
124	628897	2-(2-CHLOROETHOXY)ETHANOL	664				C4 . H9 . O2 .CL1
125 *	19615271	1-ACETYL-1,2,3,4-TETRAHYDROPYRIDINE		676			C7 . H11. N1 . O1
125	6036222	BUTYL THIAZOLE		1107			C6 . H11. N3
125	110576	1,4-DICHLORO-2-BUTENE			243	152	C4 . H6 .CL2
126	95498	%*O-CHLOROTOLUENE	817	1038			C7 . H7 .CL1
126	110930	6-METHYL-5-HEPTEN-2-ONE	68	152			C8 . H14. O1
126	124118	1-NONYLENE		402			C9 . H18
126	25447692	OCTENAL (ISOMER UNKNOWN)		637			C8 . H14. O1

† SEE FOOTNOTE ON LAST PAGE

* 2,3-DIMETHYLMALEIMIDE IS LISTED WITH MW 139 COMPOUNDS

(continued)

TABLE D1. (Continued)

IDENTIFIED COMPOUNDS BY MOLECULAR WEIGHT
NOTE--THIS LIST MAY CONTAIN COMPOUNDS THAT HAVE NOT BEEN FOUND IN ANY OF THE CONCENTRATES ANALYZED

MW	CAS NO.	COMMON NAME	DATA SET CORRELATION † DW	AWT	T4	T5	MOLECULAR FORMULA
126	77781	%DIMETHYL SULFATE		675			C2 . H6 . O4 . S1
126	53517923	1,2,4-TRIMETHYL-1,3-DIAZOCYCLOHEX-1-ENE					C7 . H14. N2
126	100447	%BENZYL CHLORIDE	887				C7 . H7 .CL1
126	4505548	3-METHYL-1,2,4-CYCLOPENTANETRIONE	892				C6 . H6 . O3
126	22287112	3-ETHYL-4-METHYL-3-PENTEN-2-ONE	506				C8 . H14. O1
126	22319251	4-METHYL-3-HEPTEN-2-ONE					C8 . H14. O1
126	3073663	1,1,3-TRIMETHYLCYCLOHEXANE	907				C9 . H18
126	1187877	5-METHYL-3-METHYLENE-2-HEXANONE	910				C8 . H14. O1
126	20685454	CIS-3,4-DIMETHYL-3-HEXEN-2-ONE	595	927			C8 . H14. O1
126	22319240	2-METHYL-2-HEPTEN-4-ONE	314				C8 . H14. O1
126	4423943	2-ETHYLCYCLOHEXANONE					C8 . H14. O1
126	1004246	4-METHYLENECYCLOHEXANEMETHANOL	500				C8 . H14. O1
126	823767	CYCLOHEXYL METHYL KETONE	434	934			C8 . H14. O1
126	1669449	3-OCTEN-2-ONE	28				C8 . H14. O1
126	513882	1,1-DICHLOROACETONE	827				C3 . H4 . O1 .CL2
126	53907612	2,4,4-TRIMETHYL-2-PENTENAL					C8 . H14. O1
126	645625	2-ETHYL-3-PROPYLACROLEIN	1109				C8 . H14. O1
126	2816571	2,6-DIMETHYLCYCLOHEXANONE	191	928			C8 . H14. O1
126	766392	3,4-DIMETHYL-2,5-FURANDIONE					C6 . H6 . O3
126	7667552	1,2,4-TRIMETHYL-CYCLOHEXANE	1023	305			C9 . H18
126	3664606	7-OCTEN-2-ONE	735				C8 . H14. O1
126	50598500	3,5,5-TRIMETHYL-2(5H)-FURANONE	940				C7 . H10. O2
126	7581977	2,3-DICHLOROBUTENE		910			C4 . H8 .CL2
126	1632264	1,2-DIAZABICYCLO[2.2.2.]OCTAN-3-ONE		898			C6 . H10. N2 . O1
126	3883587	2,2-DIMETHYL-1,3-CYCLOPENTANEDIONE	871	186	181		C7 . H10. O2
127	95512	%*O-CHLOKOANILINE		619			C6 . H6 . N1 .CL1
127	108429	%M-CHLOROANILINE	1031	437			C6 . H6 . N1 .CL1
127	3623050	HEXAHYDRO-4-METHYL-2H-AZEPIN-2-ONE		871			C7 . H13. N1 . O1
127	2314785	1-ETHYL-2,5-PYRROLIDINEDIONE	1046	873			C6 . H9 . N1 . O2
127	618428	1-ACETYLPIPERIDINE		874			C7 . H13. N1 . O1
127	458888	CONIINE					C8 . H17. N1
127	18368768	2-CHLOKO-3-PICOLINE		1072			C6 . H6 . N1 .CL1
127	29553513	3-METHYLPIPERIDINE-2,6-DIONE	2	92	80	167	C6 . H9 . N1 . O2
128	91203	%+NAPHTHALENE	527	502			C10. H8
128	74975	%CHLOROBROMOMETHANE		104			C1 . H2 .BR1 .CL1
128	62243576	2-METHYL-3-HEXENOIC ACID	468	209			C7 . H12. O2
128	106489	%*$P-CHLOROPHENOL		809			C6 . H5 . O1 .CL1
128	29901857	TRANS-3-HEPTENOIC ACID		231			C7 . H12. O2
128	13603071	%N-NITROSO-3-METHYL PIPERIDINE		1001			C6 . H12. N2 . O1
128	18292290	DIETHYLMETHYLVINYLSILANE	814	400			C7 . H16.SI1
128	106683	3-OCTANONE		229			C8 . H16. O1
128	108430	$M-CHLOROPHENOL		390			C6 . H5 . O1 .CL1
128	6945353	4,4-DIMETHYL-2-PENTENOIC ACID	321	651			C7 . H12. O2
128	15045439	2,2,5,5-TETRAMETHYL THF	96	271	68	119	C8 . H16. O1
128	79436	%BICHLORACETIC ACID					C2 . H2 . O2 .CL2

† SEE FOOTNOTE ON LAST PAGE

(Continued)

TABLE D1. (Continued)

IDENTIFIED COMPOUNDS BY MOLECULAR WEIGHT
NOTE--THIS LIST MAY CONTAIN COMPOUNDS THAT HAVE NOT BEEN FOUND IN ANY OF THE CONCENTRATES ANALYZED

MW	CAS NO.	COMMON NAME	DATA SET CORRELATION † DW	AWT	T4	T5	MOLECULAR FORMULA
128	1004291	2-BUTYL THF	309	312	129		C8 . H16. O1
128	1067205	3,3-DIETHYLPENTANE					C9 . H20
128	3074779	3-ETHYL-4-METHYLHEXANE					C9 . H20
128	26118387	3,3-DIMETHYL-2-HEXANONE		866			C8 . H16. O1
128	95578	$O-CHLOROPHENOL	938	649		180	C6 . H5 . O1 .CL1
128	98895	HEXAHYDROBENZOIC ACID	225	715			C7 . H12. O2
128	275514	%AZULENE	770				C10. H8
128	1071267	2,2-DIMETHYLHEPTANE					C9 . H20
128	2213232	2,4-DIMETHYLHEPTANE					C9 . H20
128	1072055	2,6-DIMETHYLHEPTANE					C9 . H20
128	53907725	7-OCTEN-4-OL	1103				C8 . H16. O1
128	51945983	1,5-HEPTADIENE-3,4-DIOL	78				C7 . H12. O2
128	928687	6-METHYL-2-HEPTANONE	103	909			C8 . H16. O1
128	5932912	4,4-DIMETHYLHEXANAL	875				C8 . H16. O1
128	5363644	1-(ETHENYLOXY)HEXANE	233				C8 . H16. O1
128	16747287	2,3,3-TRIMETHYLHEXANE					C9 . H20
128	5441521	3,5-DIMETHYLCYCLOHEXANOL	107				C8 . H16. O1
128	18217124	5-METHYL-2-HEPTANONE	311	921			C8 . H16. O1
128	111137	%HEXYL METHYL KETONE	680		191		C8 . H16. O1
128	541855	ETHYL AMYL KETONE	917				C8 . H16. O1
128	55670092	2-METHYLENE-1-BUTANOL ACETATE	1140				C8 . H16. O1
128	4351546	CYCLOHEXYL FORMATE	109	296			C7 . H12. O2
128	6137117	4-METHYL-3-HEPTANONE					C8 . H16. O1
128	7307020	2,4-HEPTANEDIONE	487				C7 . H12. O2
128	15120997	1-(TRIMETHYLOXIRANYL)ETHANONE	236				C7 . H12. O2
128	517237	ALPHA-ACETYLBUTYROLACTONE (GAMMA LACTONE)	562				C6 . H8 . O3
128	18409171	2-OCTEN-1-OL	563				C8 . H16. O1
128	5337724	2,6-DIMETHYLCYCLOHEXANOL	742				C8 . H16. O1
128	589639	4-OCTANONE	984				C8 . H16. O1
128	3720227	TETRAHYDRO-3,6-DIMETHYL-2H-PYRAN-2-ONE					C7 . H12. O2
128	2105400	2-METHYL-CYCLOHEXANEMETHANOL					C8 . H16. O1
128	2216344	4-METHYLOCTANE					C9 . H20
128	17429026	4-HYDROXY-4-METHYLCYCLOHEXANONE	958		154	67	C7 . H12. O2
128	15726155	3-METHYL-4-HEPTANONE	685				C8 . H16. O1
128	105215	5-PROPYLDIHYDRO-2-FURANONE		1073			C7 . H12. O2
129	1122607	NITROCYCLOHEXANE	1108				C6 . H11. N1 . O2
129	119653	%ISOQUINOLINE					C9 . H7 . N1
129	1696204	4-ACETYLMORPHOLINE	584	1064			C6 . H11. N1 . O2
129	495103	2-PHENYL ACROLEIN	699				C9 . H7 . N1
129	91225	%QUINOLINE	970	900			C9 . H7 . N1
129	42966643	N-ETHYL-4-METHYL-2-PENTANEAMINE		725			C8 . H19. N1
130	142961	%N-BUTYLETHER		791			C8 . H18. O1
130	104767	2-ETHYL-1-HEXANOL	69	168			C8 . H18. O1
130	6163662	DI-T-BUTYL ETHER		350	153		C8 . H18. O1
130	1460340	2-KETO-3-METHYL VALERIC ACID	1125	808			C6 . H10. O3

† SEE FOOTNOTE ON LAST PAGE

(Continued)

TABLE D1. (Continued)

IDENTIFIED COMPOUNDS BY MOLECULAR WEIGHT

NOTE--THIS LIST MAY CONTAIN COMPOUNDS THAT HAVE NOT BEEN FOUND IN ANY OF THE CONCENTRATES ANALYZED

MW	CAS NO.	COMMON NAME	DATA SET CORRELATION †				MOLECULAR FORMULA
			DW	AWT	T4	T5	
130	816660	2-KETOISOCAPROIC ACID	364	112			C6 . H10. O3
130	628466	5-METHYL HEXANOIC ACID	308	237			C7 . H14. O2
130	111148	%N-HEPTANOIC ACID	158	120	5	69	C7 . H14. O2
130	58973185	2-METHOXY-3-METHYLCROTONIC ACID	137	643			C6 . H10. O3
130	31367461	3-METHYL-2-HEPTANOL	870	273			C8 . H18. O1
130	1185393	2,2-DIMETHYLVALERIC ACID		119		173	C7 . H14. O2
130	19889373	2-ETHYL-2-METHYLBUTYRIC ACID		672			C7 . H14. O2
130	106707	METHYL CAPROATE	372	872			C7 . H14. O2
130	79016	%ETHYLENE TRICHLORIDE					C2 . H1 .CL3
130	4433856	2-ETHYLACETOACETIC ACID	872				C6 . H10. O3
130	1321740	DIVINYLBENZENE	444			14	C10. H10
130	447530	1,2-DIHYDRONAPHTHALENE	404				C10. H10
130	1561111	4-METHYLHEXANOIC ACID	228	46			C7 . H14. O2
130	4536236	2-METHYLCAPROIC ACID	593	243			C7 . H14. O2
130	123922	%3-METHYL-1-BUTANOL ACETATE	829				C7 . H14. O2
130	625252	2-METHYL-2-HEPTANOL	271				C8 . H18. O1
130	767599	1-METHYL INDENE	61				C10. H10
130	36687997	3-ETHOXY-3-METHYL-2-BUTANONE	484				C7 . H14. O2
130	29006006	6-METHOXY-2-HEXANONE	486	908			C7 . H14. O2
130	54630501	5-METHYL-2-HEPTANOL	220				C8 . H18. O1
130	4352981	2-METHYL-2-PROPYL-1,3-DIOXOLANE	494				C7 . H14. O2
130	111875	%N-OCTANOL	93	685			C8 . H18. O1
130	3054920	2,3,4-TRIMETHYL-3-PENTANOL	286				C8 . H18. O1
130	3730607	2,5-DIMETHYL-2-HEXANOL	291				C8 . H18. O1
130	4405167	2-METHYL-2-ISOPROPYL-1,3-DIOXOLANE	1114				C7 . H14. O2
130	108576	M-DIETHENYLBENZENE	705			15	C10. H10
130	2177471	2-METHYL INDENE					C10. H10
130	767602	3-METHYL INDENE	977				C10. H10
130	55256172	CHLOROFLUOROBENZENE	1101				C6 . H4 .CL1 . F1
130	14979396	4-METHYL-3-HEPTANOL	535				C8 . H18. O1
130	15677153	1,1A,6,6A-TETRAHYDROCYCLOPROP[A]INDENE				32	C10. H10
130	539822	ETHYLVALERATE	1003				C7 . H14. O2
130	3128061	5-OXO-HEXANOIC ACID	578				C6 . H10. O3
130	106672	2-ETHYL-4-METHYL-1-PENTANOL	153				C8 . H18. O1
130	2005	2-ETHYLVALERIC ACID		235			C7 . H14. O2
130	91190	QUINOXALINE					C8 . H6 . N2
130	53907918	2-ETHYL-5-METHYLDIOXANE		467			C7 . H14. O2
130	10150875	4-ACETYLOXY-2-BUTANONE					C6 . H10. O3
130	26952216	ISO-OCTANOL					C8 . H18. O1
131	3475636	%TRIMETHYL NITROSO UREA		455			C4 . H9 . N3 . O2
132	824635	2-METHYL INDAN	454			29	C10. H12
132	119642	TETRALIN	443	751		22	C10. H12
132	824226	4-METHYL INDAN	760	516		30	C10. H12
132	767588	1-METHYL INDAN	717	339		12	C10. H12
132	110941	%GLUTARIC ACID		573			C5 . H8 . O4

† SEE FOOTNOTE ON LAST PAGE

(Continued)

TABLE D1. (Continued)

IDENTIFIED COMPOUNDS BY MOLECULAR WEIGHT
NOTE--THIS LIST MAY CONTAIN COMPOUNDS THAT HAVE NOT BEEN FOUND IN ANY OF THE CONCENTRATES ANALYZED

MW	CAS NO.	COMMON NAME	DATA SET CORRELATION † DW	AWT	T4	T5	MOLECULAR FORMULA
132	83330	1-INDANONE	1118	587		42	C9 . H8 . O1
132	111897	1,5-DIMETHOXYPENTANE		625			C7 . H16. O2
132	874351	5-METHYL INDAN	456	1012		5	C10. H12
132	5379204	3,5-DIMETHYL STYRENE		132			C10. H12
132	2039896	2,5-DIMETHYL STYRENE		655			C10. H12
132	104552	%CINNAMALDEHYDE	982	486			C9 . H8 . O1
132	71556	%METHYL CHLOROFORM		276			C2 . H3 .CL3
132	1560061	CROTONYLBENZENE	1152				C10. H12
132	768490	(2-METHYL-1-PROPENYL)BENZENE	767				C10. H12
132	2039909	2,6-DIMETHYLSTYRENE	1044	770			C10. H12
132	7525624	3-ETHYLSTYRENE	186			4	C10. H12
132	3454077	4-ETHYLSTYRENE	166	1096	233	2	C10. H12
132	1587048	O-ALLYLTOLUENE	713				C10. H12
132	55724044	5-METHOXY-2-METHYL-2-PENTANOL	551				C7 . H16. O2
132	115764	2,2-DIETHYLPROPYLENE GLYCOL	105	729			C7 . H16. O2
132	762469	1-METHYLHEXYLHYDROPEROXIDE	283				C7 . H16. O2
132	7564638	O-ETHYLSTYRENE	986	1048		27	C10. H12
132	1195320	P-ISOPROPENYLTOLUENE					C10. H12
132	20225245	2-ETHYL PENTANOIC ACID	1087				C7 . H14. O2
132	33877871	1,2,3,3A-TETRAHYDRO AZULENE	1021				C10. H12
132	53907952	1-(1-METHYLPROPOXY)-2-PROPANOL	8				C7 . H16. O2
132	5086	PROPYLENE GLYCOL MONOBUTYL ETHER			146		C7 . H16. O2
132	8898	7-METHYLBENZOFURAN					C9 . H8 . O1
133	13351730	2-METHYLBENZOTRIAZOLE	657				C7 . H7 . N3
134	1074437	1-METHYL-3-PROPYL BENZENE		998			C10. H14
134	135988	SEC-BUTYL BENZENE		783		47	C10. H14
134	2870044	2-ETHYL-1,3-DIMETHYL BENZENE		338			C10. H14
134	934805	4-ETHYL-1,2-DIMETHYL BENZENE	1091	184	227	49	C10. H14
134	1758889	2-ETHYL-1,4-DIMETHYL BENZENE		615	231		C10. H14
134	527844	2-ISOPROPYL TOLUENE (O-CYMENE)					C10. H14
134	934747	1-ETHYL-3,5-DIMETHYL BENZENE	1090	341	222		C10. H14
134	141935	1,3-DIETHYL BENZENE	131	772		3	C10. H14
134	1074175	1-METHYL-2-PROPYL BENZENE		515	224		C10. H14
134	135013	1,2-DIETHYL BENZENE	133			9	C10. H14
134	104518	N-BUTYLBENZENE		525			C10. H14
134	874419	1-ETHYL-2,4-DIMETHYL BENZENE		521	232		C10. H14
134	105055	1,4-DIETHYL BENZENE	132	187		8	C10. H14
134	488233	1,2,3,4-TETRAMETHYL BENZENE		754			C10. H14
134	95932	DURENE		549			C10. H14
134	933982	1-ETHYL-2,3-DIMETHYL BENZENE	1042	522			C10. H14
134	527537	ISODURENE	1092	189			C10. H14
134	629061	1-CHLOROHEPTANE		508			C7 . H15.CL1
134	7169348	BENZOFURANONE		365			C8 . H6 . O2
134	98066	TERT-BUTYLBENZENE		979			C10. H14
134	111900	DIETHYLENE GLYCOL, MONOMETHYL ETHER (CARBITOL)	194	371			C6 . H14. O3

† SEE FOOTNOTE ON LAST PAGE

(Continued)

TABLE D1. (Continued)

IDENTIFIED COMPOUNDS BY MOLECULAR WEIGHT

NOTE--THIS LIST MAY CONTAIN COMPOUNDS THAT HAVE NOT BEEN FOUND IN ANY OF THE CONCENTRATES ANALYZED

MW	CAS NO.	COMMON NAME	DATA SET CORRELATION † DW	AWT	T4	T5	MOLECULAR FORMULA
134	538932	ISOBUTYL BENZENE		971			C10. H14
134	1074551	1-METHYL-4-PROPYLBENZENE		524	221		C10. H14
134	99876	%P-CYMENE (P-ISOPROPYL TOLUENE)	1068	188			C10. H14
134	535773	META-CYMENE (M-ISOPROPYL TOLUENE)	1124	972			C10. H14
134	200	DIMETHYL ETHYL BENZENE		550	225		C10. H14
134	201	DIMETHYL ETHYL BENZENE		551	226		C10. H14
134	202	DIMETHYL ETHYL BENZENE		973			C10. H14
134	104541	%CINNAMYL ALCOHOL		988			C9 . H10. O1
134	205	METHYL-N-PROPYLBENZENE		631			C10. H14
134	206	METHYL-N-PROPYLBENZENE		632			C10. H14
134	208	CYMENE (ISOMER UNKNOWN)		838			C10. H14
134	209	CYMENE (ISOMER UNKNOWN)		839			C10. H14
134	87412	PHTHALIDE	241	247		149	C8 . H6 . O2
134	106627	2-(2-HYDROXYPROPOXY)-1-PROPANOL (A DIPROPYLENE GLYCOL)	397	274			C6 . H14. O3
134	53951501	ETHYLBENZALDEHYDE	184		113	53	C9 . H10. O1
134	4748781	P-ETHYLBENZALDEHYDE	445				C9 . H10. O1
134	5779942	2,5-DIMETHYLBENZALDEHYDE	208				C9 . H10. O1
134	49826542	2,3-BIS(METHYLENE)-BICYCLO(3.2.1)OCTANE					C10. H14
134	103797	BENZYL METHYL KETONE	214				C9 . H10. O1
134	577162	2'-METHYLACETOPHENONE	446				C9 . H10. O1
134	767986	1,4-DIHYDRO-1-METHYL-4-OXONICOTINONITRILE	826				C7 . H6 . N2 . O1
134	2085883	%2-METHYL-2-PHENYLOXIRANE	862				C9 . H10. O1
134	93550	%PROPIOPHENONE	935		157		C9 . H10. O1
134	26444199	1-(METHYLPHENYL)ETHANONE	369				C9 . H10. O1
134	621636	2,2-DIETHOXYETHANOL	840				C6 . H14. O3
134	122009	P-METHYL ACETOPHENONE					C9 . H10. O1
134	5973717	3,4-DIMETHYLBENZALDEHYDE	865				C9 . H10. O1
134	110985	DIPROPYLENE GLYCOL	972			188	C6 . H14. N3
134	6628804	2-CHLOROCYCLOHEXANOL					C6 . H11. O1 .CL1
134	29538770	TRANS-4-CHLOROCYCLOHEXANOL					C6 . H11. O1 .CL1
134	95158	BENZOTHIOPHENE		1094			C8 . H6 . S1
135	95169	BENZOTHIAZOLE	467	155		155	C7 . H5 . N1 . S1
135	272162	1,2-BENZISOTHIAZOLE		494			C7 . H5 . N1 . S1
135	99036	%M-AMINOACETOPHENONE	820				C8 . H9 . N1 . O1
135	103833	N,N-DIMETHYLBENZYLAMINE	855	903			C9 . H13. N1
135	36917369	4-ETHYL-2,6-DIMETHYL PYRIDINE		1058			C9 . H13. N1
135	94699	N-(2-METHYLPHENYL)FORMAMIDE		705			C8 . H9 . N1 . O1
135	103844	N-PHENYL ACETAMIDE	852		74	181	C8 . H9 . N1 . O1
135	6086	2-METHYLBENZAMIDE		995			C8 . H9 . N1 . O1
136	118901	ORTHO-TOLUIC ACID	221	30	48	120	C8 . H8 . O2
136	93583	%METHYL BENZOATE	9	553	13	16	C8 . H8 . O2
136	103822	%PHENYLACETIC ACID	49	35	69	61	C8 . H8 . O2
136	99047	M-TOLUIC ACID	72	15	121	103	C8 . H8 . O2
136	99945	P-TOLUIC ACID	73	42	128	104	C8 . H8 . O2
136	138863	1-METHYL-4-(1-METHYLETHENYL)-CYCLOHEXENE		854			C10. H16

† SEE FOOTNOTE ON LAST PAGE

(Continued)

TABLE D1. (Continued)

IDENTIFIED COMPOUNDS BY MOLECULAR WEIGHT
NOTE--THIS LIST MAY CONTAIN COMPOUNDS THAT HAVE NOT BEEN FOUND IN ANY OF THE CONCENTRATES ANALYZED

MW	CAS NO.	COMMON NAME	DATA SET CORRELATION †				MOLECULAR FORMULA
			DW	AWT	T4	T5	
136	764592	4-ETHYLBENZYL ALCOHOL	764				C9 . H12. O1
136	617947	%2-PHENYLISOPROPANOL	226	686			C9 . H12. O1
136	63142436	3,5-NONADIEN-7-YL-2-OL					C9 . H12. O1
136	536505	P,ALPHA-DIMETHYLBENZYL ALCOHOL	323				C9 . H12. O1
136	591311	M-ANISALDEHYDE	1122				C8 . H8 . O2
136	7339479	4-HYDROXYACETOPHENONE				150	C8 . H8 . O2
136	4013347	1-METHOXYETHYLBENZENE					C9 . H12. O1
136	99843	4-METHYLENE-1-(1-METHYLETHYL)CYCLOHEXENE			182		C10. H16
136	622855	PHENYLPROPYL ETHER		1093			C9 . H12. O1
137	118923	%ANTHRANILIC ACID	395	477			C7 . H7 . N1 . O2
137	520696	3-ETHYL-2,4,5-TRIMETHYL-1H-PYRROLE					C9 . H15. N1
137	88722	O-NITROTOLUENE			64	78	C7 . H7 . N1 . O2
137	99990	P-NITROTOLUENE			194		C7 . H7 . N1 . O2
138	471012	3,5,5-TRIMETHYLCYCLOHEX-3-EN-1-ONE		372			C9 . H14. O1
138	99098	%*M-NITROANILINE		996			C6 . H6 . N2 . O2
138	78591	*ISOPHORONE	75	230		76	C9 . H14. O1
138	69727	%SALICYLIC ACID	47	110	143	106	C7 . H6 . O3
138	17299411	3,4,4-TRIMETHYL-2-CYCLOHEXEN-1-ONE	698	822			C9 . H14. O1
138	17429297	4,4,5-TRIMETHYL-2-CYCLOHEXEN-1-ONE	968	384			C9 . H14. O1
138	286768	BICYCLO DECANE		626			C10. H18
139	622253	CHLOROVINYLBENZENE	644	993			C8 . H7 . CL1
138	493016	DECALIN	607				C10. H18
139	13747734	2-(1-METHYLETHYLIDENE)CYCLOHEXANONE	325				C9 . H14. O1
138	14377118	1-(1-CYCLOHEPTEN-1-YL)ETHANONE	889				C9 . H14. O1
138	55282901	3,8-NONADIEN-2-ONE	918				C9 . H14. O1
138	93561	%STYRENE GLYCOL					C8 . H10. O2
138	874600	1-CYCLOHEXYLIDENE ACETONE					C9 . H14. O1
139	623814	%DIETHYL SULFITE	1028				C4 . H10. O3 . S1
138	54955	PENTYLENETETRAZOLE	365				C6 . H10. N4
138	13837713	M-MENTH-1(7)-ENE (R)-(-)	1051				C10. H18
138	122996	2-PHENOXYETHANOL	398				C8 . H10. O2
139	768503	1-(1-CYCLOHEXEN-1-YL)-2-PROPANONE		595			C9 . H14. O1
138	151100	1,3-DIMETHOXYBENZENE					C8 . H10. O2
138	8997	3,4-DIHYDROXYBENZALDEHYDE	576				C7 . H6 . O3
139	100027	%*P-NITRO PHENOL		1069			C6 . H5 . N1 . O3
139	21150016	BETA,BETA-DIMETHYL HISTAMINE		1024			C7 . H13. N3
139	20189428	3-ETHYL-4-METHYL-1H-PYRROLE-2,5-DIONE	195				C7 . H9 . N1 . O2
125	17825864	2,3-dimethylmaleimide	196				C6 . H7 . N1 . O2
139	3717155	4-METHYLBENZALDEHYDE OXIME			192		C8 . H9 . N1 . O1
140	1674335	1,2-DICHLOROPENTANE		507			C5 . H10.CL2
140	873949	3,3,5-TRIMETHYCYCLOHEXANONE	811	792			C9 . H16. O1
140	872059	DECYLENE		251			C10. H20
140	17773669	2,2-DICHLORO-3-METHYLBUTANE	628	665			C5 . H10.CL2
140	16525056	2,6-DIMETHYL-2-HEPTEN-4-ONE		609			C9 . H16. O1
140	4342603	4-METHYL-3-CYCLOHEXENE-1-CARBOXYLIC ACID		671			C8 . H12. O2

† SEE FOOTNOTE ON LAST PAGE

(Continued)

TABLE D1. (Continued)

IDENTIFIED COMPOUNDS BY MOLECULAR WEIGHT

NOTE--THIS LIST MAY CONTAIN COMPOUNDS THAT HAVE NOT BEEN FOUND IN ANY OF THE CONCENTRATES ANALYZED

MW	CAS NO.	COMMON NAME	DATA SET CORRELATION † DW	AWT	T4	T5	MOLECULAR FORMULA
140	507459	AMYLENE DICHLORIDE	39	743			C5 . H10.CL2
140	23010073	1,3-DICHLORO-2-METHYLBUTANE (A DICHLOROPENTANE)	249				C5 . H10.CL2
140	2408379	2,2,6-TRIMETHYLCYCLOHEXANONE	516				C9 . H16. O1
140	625672	2,4-DICHLOROPENTANE	883				C5 . H10.CL2
140	3508789	3-ALLYL-2,4-PENTANEDIONE	897				C8 . H12. O2
140	33046810	7-METHYL-3-OCTEN-2-ONE	899				C9 . H16. O1
140	1920214	3,4-DIHYDRO-2,5-DIMETHYL-2H-PYRAN-2-CARBOXALDEHYDE	613				C8 . H12. O2
140	3552338	3-ETHYL-4-METHYL-2,5-FURANDIONE	29				C7 . H8 . O3
140	1561202	3,3-DICHLORO-2-PROPENOIC ACID	844				C3 . H2 . O2 .CL2
140	1678984	ISOBUTYLCYCLOHEXANE					C10. H20
140	10141227	2,3-DICHLOROISOBUTANAL	824				C4 . H6 . O1 .CL2
140	3664753	(2,2-DIMETHYLCYCLOPENTYL) ETHANONE					C9 . H16. O1
140	7058051	1-ETHYL-2,3-DIMETHYLCYCLOHEXANE					C10. H20
140	94655	2-PROPYLCYCLOHEXANONE	736				C9 . H16. O1
140	89963	1-CHLORO-2-ETHYLBENZENE	641				C8 . H9 .CL1
140	1689787	2-ISOPROPYLTHIOPHENE		690			C8 . H12. S1
140	5009325	8-NONENE-2-ONE	1000	501			C9 . H16. O1
140	16523061	CYCLOPENTANE CARBOXYLIC ACID, VINYL ESTER		734			C8 . H12. O2
140	126818	DIMETHYLCYCLOHEXANE DIONE		904			C8 . H12. O2
140	7180623	4-METHOXY-5-METHYL-4-CYCLOPENTEN-1,3-DIONE		704			C7 . H8 . O3
140	2463538	2-NONENAL		1	29	166	C9 . H16. O1
140	8896	2,3-DICHLOROACRYLIC ACID	577				C3 . H2 . O2 .CL2
141	77678	%ETHOSUXIMIDE	298	38			C7 . H11. N1 . O2
141	3470971	N-PROPYLSUCCINAMIDE		416			C7 . H11. N1 . O2
141	5809416	HEXAMETHYLENE ACETAMIDE		1031			C8 . H15. N1 . O1
141	1124534	N-ACETYLCYCLOHEXYLAMINE		316			C8 . H15. N1 . O1
142	90120	%1-METHYLNAPHTHALENE	206	517		57	C11. H10
142	91576	%2-METHYLNAPHTHALENE	169	340	234	56	C11. H10
142	1577191	3-OCTENOIC ACID	478	367			C8 . H14. O2
142	75990	%DALAPON	387	576			C3 . H4 . O2 .CL2
142	124185	%DECANE					C10. H22
142	1072168	2,7-DIMETHYLOCTANE					C11. H22
142	108838	DIISOBUTYL KETONE	217	1027		41	C9 . H18. O1
142	24628368	4,6,6-TRIMETHYLTETRAHYDRO-2-PYRANONE	558	393			C8 . H14. O2
142	585251	2,3-OCTANEDIONE	520				C8 . H14. O2
142	111444	%+$DICHLOROETHYL ETHER	335		189	136	C4 . H8 . O1 .CL2
142	40991933	2-METHYLCYCLOPENTANOL ACETATE	1131				C8 . H14. O2
142	249189	2-HEXEN-1-OL	920				C8 . H14. O2
142	55956371	4,5-DIMETHYL-2-HEPTEN-3-OL	310				C9 . H18. O1
142	622457	%CYCLOHEXYL ACETATE	294				C8 . H14. O2
142	116541	METHYL DICHLOROACETATE	950	933			C3 . H4 . O2 .CL2
142	36712206	TRANS-3-BUTYLTETRAHYDRO-2-METHYLFURAN	780				C9 . H18. O1
142	815247	2,2,4,4-TETRAMETHYL-3-PENTANONE					C9 . H18. O1
142	124196	NONANAL					C9 . H18. O1
142	623121	P-CHLOROANISOLE	1160				C7 . H7 . O1 .CL1

† SEE FOOTNOTE ON LAST PAGE

(Continued)

TABLE D1. (Continued)

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IDENTIFIED COMPOUNDS BY MOLECULAR WEIGHT
NOTE--THIS LIST MAY CONTAIN COMPOUNDS THAT HAVE NOT BEEN FOUND IN ANY OF THE CONCENTRATES ANALYZED

MW	CAS NO.	COMMON NAME	DATA SET CORRELATION †				MOLECULAR FORMULA
			DW	AWT	T4	T5	
142	4621049	4-ISOPROPYLCYCLOHEXANOL	534				C9 . H18. O1
142	18294898	4-OCTENOIC ACID	1017	391			C8 . H14. O2
142	4331548	4-METHYLCYCLOHEXANE CARBOXYLIC ACID	1009				C8 . H14. O2
142	2051301	2,6-DIMETHYLOCTANE					C10. H22
142	1540381	3-ISOPROPYL-2,4-PENTANEDIONE	1030				C8 . H14. O1
142	4032933	2,3,6-TRIMETHYLHEPTANE		1036			C10. H22
142	34003775	5-BUTYLDIHYDRO-2-FURANONE		394			C8 . H14. O2
143	91598	%*2-NAPHTHYLAMINE					C10. H9 . N1
143	20193231	N-PROPYL-1-HEXANAMINE	1001	495			C9 . H21. N1
143	1721933	1-METHYLISOQUINOLINE	700				C10. H9 . N1
143	491350	%P-TOLUQUINONE	1055				C10. H9 . N1
143	1125400	%M-TOLUQUINONE	1008				C10. H7 . N1
143	91634	%QUINAIDINE	971	1065			C10. H9 . N1
143	115673	5-METHYL-5-ETHYL-2,4-OXAZOLIDINEDIONE		915			C6 . H9 . N1 . O3
144	124072	%CAPRYLIC ACID	48	33	109	184	C8 . H16. O2
144	149575	2-ETHYLHEXANOIC ACID	71	9	4	161	C8 . H16. O2
144	2233003	3,3,3-TRICHLOROPROPENE	117	978			C3 . H3 .CL3
144	1014	3-METHOXY-2-METHYL-2-PENTENOIC ACID	623	433			C7 . H12. O3
144	786	ETHYL HEXANOIC ACID					C8 . H16. O2
144	785	ETHYL HEXANOIC ACID					C8 . H16. O2
144	41065912	3-ETHYLHEXANOIC ACID	1111	107			C8 . H16. O2
144	1188029	2-METHYLHEPTANOIC ACID	316	113			C8 . H16. O2
144	109217	BUTYL BUTYRATE		117			C8 . H16. O2
144	819976	2-BUTYL-N-BUTYRATE	615	70			C8 . H16. O2
144	1008	2-METHOXY-3-METHYL-2-PENTENOIC ACID	587	419			C7 . H12. O3
144	1009	2-METHOXY-4-METHYL-2-PENTENOIC ACID	299	262			C7 . H12. O3
144	1124136	~~1,2-CYCLOBUTANEDICARBOXYL~~ USE CAS NO. 488211, NEXT PAGE	~~14~~	~~275~~			~~C6 . H8 . O4~~
144	41654840	4-KETOISOHEPTANOIC ACID	544	652			C7 . H12. O3
144	2567148	1,1,3-TRICHLORO-1-PROPENE	428	1021		133	C3 . H3 .CL3
144	21400259	1,1,2-TRICHLORO-1-PROPENE	869		211		C3 . H3 .CL3
144	18636550	1,1-DIMETHYL INDENE	1015				C11. H12
144	6299667	4-ETHYLHEXANOIC ACID	598				C8 . H16. O2
144	1573280	3,6-DIMETHYL-3-HEPTANOL	884				C9 . H20. O1
144	19424294	4,4,5,5-TETRAMETHYL-1,3-DIOXOLAN-2-ONE	324				C7 . H12. O3
144	97870	BUTYL ISOBUTYRATE	313				C8 . H16. O2
144	19549770	2,4-DIMETHYL-4-HEPTANOL	591				C9 . H20. O1
144	637649	TETRAHYDROFURFURYL ACETATE	1141				C7 . H12. O3
144	5185977	5-(ACETYLOXY)-2-PENTANONE	1143	1084			C7 . H12. O3
144	933404	1,1-DIMETHOXYCYCLOHEXANE	1145				C8 . H16. O2
144	623938	5-NONANOL	1147				C9 . H20. O1
144	53264572	1,2-DIMETHYL INDENE					C11. H12
144	5932796	4-NONANOL	239				C9 . H20. O1
144	17429059	6-METHOXY-2-METHYL-3-HEXANONE	507				C8 . H16. O2
144	19549736	2,6-DIMETHYL-3-HEPTANOL	508				C9 . H20. O1
144	19780406	5-ETHYL-2-HEPTANOL	280				C9 . H20. O1

† SEE FOOTNOTE ON LAST PAGE

(Continued)

TABLE D1. (Continued)

IDENTIFIED COMPOUNDS BY MOLECULAR WEIGHT

NOTE--THIS LIST MAY CONTAIN COMPOUNDS THAT HAVE NOT BEEN FOUND IN ANY OF THE CONCENTRATES ANALYZED

MW	CAS NO.	COMMON NAME	DATA SET CORRELATION † DW	AWT	T4	T5	MOLECULAR FORMULA
144	6135542	2-T-BUTYL-2-METHYL-1,3-DIOXOLANE	556				C8 . H16. O2
144	62238022	2-BUTOXYPENTANE	561				C9 . H20. O1
144	42329908	2,4-DIMETHYL HEXANOIC ACID	794				C8 . H16. O2
144	54004421	2,3-DIMETHYL-BUTANOIC ACID, ETHYL ESTER					C8 . H16. O2
144	123660	%ETHYL HEXANOATE	1004				C8 . H16. O2
144	488211	2,3-DIMETHYLMALEIC ACID	14	50	19	35	C6 . H8 . O4
144	25713375	~~2,3-DIMETHYLMALEIC ACID~~ USE CAS NO. 488211, ABOVE					C6 . H8 . O4
144	106736	METHYL HEPTANOATE	149				C8 . H16. O2
144	90153	1-NAPHTHALENOL					C10. H8 . O1
144	5340363	3-METHYL-3-OCTANOL		1076			C9 . H20. O1
144	144	2-METHOXY-2-HEXENOIC ACID		737			C7 . H12. O3
144	5087	2-ACETYL-3-METHYLBUTANOIC ACID					C7 . H12. O3
145	19064698	AMINOPHTHALAZINE		574			C8 . H7 . N3
146	4912929	1,1-DIMETHYLINDAN					C11. H14
146	1680519	6-METHYL TETRALIN	721	336			C11. H14
146	4175535	1,3-DIMETHYL INDAN					C11. H14
146	2809645	5-METHYL TETRALIN	1072	765			C11. H14
146	1075225	5,6-DIMETHYL INDAN					C11. H14
146	17059482	1,6-DIMETHYL INDAN		963			C11. H14
146	17057828	1,2-DIMETHYL INDAN	1093	964			C11. H14
146	95501	%+$O-DICHLORO BENZENE	143	528	24	74	C6 . H4 .CL2
146	96184	%TRICHLOROPROPANE	44	558			C3 . H5 .CL3
146	3877198	2-METHYL TETRALIN	976	345			C11. H14
146	6682719	4,7-DIMETHYL INDAN		532			C11. H14
146	106467	%*+$P-DICHLOROBENZENE	340	834	63	194	C6 . H4 .CL2
146	617	DIMETHYL INDAN		763			C11. H14
146	616	DIMETHYL INDAN		533			C11. H14
146	615	DIMETHYL INDAN	1120	529			C11. H14
146	626517	3-METHYLGLUTARIC ACID		575			C6 . H10. O4
146	124049	%ADIPIC ACID		222			C6 . H10. O4
146	1001	1-SEC-BUTOXY-2-METHOXYPROPANE		382			C8 . H18. O2
146	541731	%+$M-DICHLOROBENZENE	651	616	188	134	C6 . H4 .CL2
146	1559815	1-METHYL TETRALIN	947	1013			C11. H14
146	1012	1,3-PROPYLENE GLYCOL, BUTYL METHYL DIETHER		431			C8 . H18. O2
146	28715266	4,7-DIMETHYLBENZOFURAN		828			C10. H10. O1
146	617629	2-METHYLGLUTARIC ACID		236			C6 . H10. O4
146	4830993	1-ETHYL INDAN	718				C11. H14
146	56147638	2-ETHYL INDAN	212				C11. H14
146	122576	BENZILIDENEACETONE	761			153	C10. H10. O1
146	598776	1,1,2-TRICHLOROPROPANE	1168				C3 . H5 .CL3
146	597433	2,2-DIMETHYLSUCCINIC ACID	779				C6 . H10. O4
146	52689244	5-ETHYL INDAN					C11. H14
146	4489843	(3-METHYL-2-BUTENYL)BENZENE					C11. H14
146	6072577	2,3-DIHYDRO-3-METHYL-1H-INDEN-1-ONE					C10. H10. O1
146	3658955	1,1-DIETHOXYBUTANE					C8 . H18. O2

† SEE FOOTNOTE ON LAST PAGE

(Continued)

TABLE D1. (Continued)

IDENTIFIED COMPOUNDS BY MOLECULAR WEIGHT

NOTE--THIS LIST MAY CONTAIN COMPOUNDS THAT HAVE NOT BEEN FOUND IN ANY OF THE CONCENTRATES ANALYZED

MW	CAS NO.	COMMON NAME	DATA SET CORRELATION † DW	AWT	T4	T5	MOLECULAR FORMULA
146	19947229	(1-ETHYL-2-PROPENYL)-BENZENE	1043			51	C11. H14
146	529340	3,4-DIHYDRO-1(2H)-NAPHTHALENONE				80	C10. H10. O1
146	37442550	1-PHENYL-3-BUTEN-2-ONE	706			94	C10. H10. N1
146	6705891	2,2'-BI-1,3-DIOXOLANE	709		107		C6 . H10. O4
146	54063182	(2-ETHOXY-1-METHOXYETHOXY)-ETHENE	401				C7 . H14. O3
146	328507	ALPHA-KETOGLUTARIC ACID	956				C5 . H5 . O5
146	106650	SUCCINIC ACID, DIMETHYL ESTER	366				C6 . H10. O4
146	54063148	4,4,5-TRIMETHYL-1,3-DIOXAN-1-OL		948			C7 . H14. O3
146	144194	2,2,4-TRIMETHYL-1,3-PENTANEDIOL		905			C8 . H18. O2
146	146	4-ISOPROPOXYBUTYRIC ACID		695			C7 . H14. O3
146	94962	2-ETHYL-1,3-HEXANEDIOL		466			C8 . H18. O2
146	5080	A PENTENYLBENZENE				31	C11. H14
146	769255	2,4,6-TRIMETHYLSTYRENE				13	C11. H14
146	1117868	1,2-OCTANEDIOL			27		C8 . H18. O2
147	85416	ISOINDOLE-1,3-DIONE		680			C8 . H5 . N1 . O2
148	98511	1-METHYL-4-TERT-BUTYLBENZENE					C11. H16
148	538681	AMYL BENZENE		1011			C11. H16
148	2049947	ISOPENTYLBENZENE					C11. H16
148	3968852	(2-METHYLBUTYL) BENZENE					C11. H16
148	1196583	3-PHENYLPENTANE					C11. H16
148	4132723	1,4-DIMETHYL-2-ISOPROPYL BENZENE					C11. H16
148	17851273	2,4,5-TRIMETHYLETHYL BENZENE		842			C11. H16
148	25550134	DIETHYL TOLUENE	1006	843		10	C11. H16
148	54120626	1,2,4-TRIMETHYL ETHYL BENZENE		841			C11. H16
148	2049958	(1,1-DIMETHYLPROPYL)BENZENE	716	544		48	C11. H16
148	1007267	NEOPENTYL BENZENE		958			C11. H16
148	2719520	2-PHENYLPENTANE		526			C11. H16
148	4481305	(1,2-DIMETHYLPROPYL)-BENZENE					C11. H16
148	13429077	DIPROPYLENE GLYCOL METHYL ETHER (1-(2-METHOXYPROPOXY)-2-PROPANOL)	461	156	142		C7 . H16. O3
148	55956213	2-(2-METHOXY-1-METHYLETHOXY)-1-PROPANOL	509	220			C7 . H16. O3
148	20324327	1-(2-METHOXY-1-METHYLETHOXY)-2-PROPANOL (A DIPROPYLENE GLYCOL)	227	739			C7 . H16. O3
148	55956224	2-(2-METHOXY-1-METHYLETHOXY)-2-PROPANOL	232	388			C7 . H16. O3
148	426	DIPROPYLENE GLYCOL, METHYL ETHER	250	63		118	C7 . H16. O3
148	425	DIPROPYLENE GLYCOL, METHYL ETHER	126	61		65	C7 . H16. O3
148	100	METHYLISOBUTYL BENZENE	733	756		90	C11. H16
148	108	DIETHYL TOLUENE		761			C11. H16
148	105	DIMETHYL ISOPROPYL BENZENE		762		191	C11. H16
148	104	DIMETHYL ISOPROPYL BENZENE		762	210	101	C11. H16
148	103	DIMETHYL ISOPROPYL BENZENE	1116	530	92	112	C11. H16
148	114	ETHYL TRIMETHYL BENZENE		531			C11. H16
148	113	ETHYL TRIMETHYL BENZENE		750			C11. H16
148	121	C5 BENZENE		527			C11. H16
148	120	C5 BENZENE		344			C11. H16
148	119	C5 BENZENE		759			C11. H16
148	118	C5 BENZENE		757			C11. H16

† SEE FOOTNOTE ON LAST PAGE

(Continued)

TABLE D1. (Continued)

WATER POLLUTANTS PAGE 21

IDENTIFIED COMPOUNDS BY MOLECULAR WEIGHT

NOTE--THIS LIST MAY CONTAIN COMPOUNDS THAT HAVE NOT BEEN FOUND IN ANY OF THE CONCENTRATES ANALYZED

MW	CAS NO.	COMMON NAME	DATA SET CORRELATION † DW	AWT	T4	T5	MOLECULAR FORMULA
148	115208	%2,2,2-TRICHLOROETHANOL	583	646			C2 . H3 . O1 .CL3
148	13588288	2-(2-METHOXYPROPOXY)-1-PROPANOL (A DIPROPYLENE GLYCOL, ME)		272			C7 . H16. O3
148	4218488	P-ETHYL-ISOPROPYLBENZENE	714	1019		11	C11. H16
148	669045	7-METHYL-3(2H)-BENZOFURANONE		660			C9 . H8 . O2
148	20895414	6-METHYL-3(2H)-BENZOFURANONE	902	438			C9 . H8 . O2
148	3453643	3-METHYL PHTHALIDE		659			C9 . H8 . O2
148	137439	CYCLOPENTYL BROMIDE	627				C5 . H9 .BR1
148	89747	2',4'-DIMETHYLACETOPHENONE	451				C10. H12. O1
148	487683	2,4,6-TRIMETHYLBENZALDEHYDE	1121				C10. H12. O1
148	5779726	2,4,5-TRIMETHYLBENZALDEHYDE	1064				C10. H12. O1
148	579077	1-PHENYL-1,2-PROPANEDIONE	1157				C9 . H8 . O2
148	937304	%4'-ETHYLACETOPHENONE	58			95	C10. H12. O1
148	2142714	2',3'-DIMETHYLACETOPHENONE	185				C10. H12. O1
148	2142645	2'-ETHYLACETOPHENONE	70			55	C10. H12. O1
148	1002671	DIETHYLENE GLYCOL, METHYL ETHYL DIETHER	315				C7 . H16. O3
148	54120648	5-METHYL-1(3H)-ISOBENZOFURANONE	504	606			C9 . H8 . O2
148	18328115	PHENYLBUTANAL	911				C10. H12. O1
148	122032	P-ISOPROPYLBENZALDEHYDE; CUMINALDEHYDE	501				C10. H12. O1
148	4706892	2,4-DIMETHYLISOPROPYLBENZENE					C11. H16
148	104461	ANETHOLE					C10. H12. O1
148	5779748	3,4,5-TRIMETHYLBENZALDEHYDE					C10. H12. O1
148	85449	PHTHALIC ANHYDRIDE	15	315			C8 . H4 . O3
148	4920994	M-ETHYLISOPROPYLBENZENE	715				C11. H16
148	4706905	1,3-DIMETHYL-5-(1-METHYLETHYL)-BENZENE					C11. H16
148	2142769	2,6-DIMETHYL ACETOPHENONE	430				C10. H12. O1
148	22699703	3-ETHYLACETOPHENONE	413				C10. H12. O1
148	5161046	P-ISOBUTYLTOLUENE	751				C11. H16
148	700129	PENTAMETHYLBENZENE					C11. H16
148	1075496	4-ETHENYL BENZOIC ACID					C9 . H8 . O2
148	137	5,5-DIMETHYLFURANONE		936			C6 . H8 . O2
148	1007325	1-PHENYL-2-BUTANONE		604			C10. H12. O1
148	529339	1,2,3,4-TETRAHYDRO-1-NAPHTHALENONE				146	C10. H12. O1
149	537928	%M-ACETOTOLUIDE		825			C9 . H11. N1 . O1
149	91667	N,N-DIETHYLANILINE		1062			C10. H15. N1
150	499752	%CARVACROL		749			C10. H14. O1
150	18309325	VERBENONE					C10. H14. O1
150	499069	3,5-DIMETHYLBENZOIC ACID	216	36	124		C9 . H10. O2
150	501520	%HYDROCINNAMIC ACID	222	201	123	105	C9 . H10. O2
150	611018	2,4-DIMETHYLBENZOIC ACID	64	12	133	123	C9 . H10. O2
150	610720	2,5-DIMETHYLBENZOIC ACID	589	41			C9 . H10. O2
150	122601	%GLYCIDYL PHENYL ETHER		827			C9 . H10. O2
150	585342	META-TERT-BUTYLPHENOL		622			C10. H14. O1
150	98544	%P-TERT-BUTYL PHENOL	878	429			C10. H14. O1
150	632462	2,6-DIMETHYLBENZOIC ACID	77	238			C9 . H10. O2
150	603792	2,3-DIMETHYLBENZOIC ACID	189	124			C9 . H10. O2

† SEE FOOTNOTE ON LAST PAGE

(Continued)

TABLE D1. (Continued)

IDENTIFIED COMPOUNDS BY MOLECULAR WEIGHT

NOTE--THIS LIST MAY CONTAIN COMPOUNDS THAT HAVE NOT BEEN FOUND IN ANY OF THE CONCENTRATES ANALYZED

MW	CAS NO.	COMMON NAME	DATA SET CORRELATION †				MOLECULAR FORMULA
			DW	AWT	T4	T5	
150	492375	2-PHENYLPROPIONIC ACID	845	16	122	121	C9 . H10. O2
150	3299056	(1-ETHOXYETHYL)BENZENE	381				C10. H14. O1
150	88186	O-TERT-BUTYLPHENOL		798			C10. H14. O1
150	93890	%ETHYL BENZOATE	336		218	52	C9 . H10. O2
150	619045	3,4-DIMETHYLBENZOIC ACID	223	109	7		C9 . H10. O2
150	119675	2-FORMYLBENZOIC ACID					C8 . H6 . O3
150	1809105	3-BROMOPENTANE		1092			C5 . H11.BR1
150	28134318	O-ETHYLBENZOIC ACID	334	48	36	88	C9 . H10. O2
150	101417	PHENYL ACETIC ACID, METHYL ESTER	149				C9 . H10. O2
150	26967657	DIETHYL PHENOL,(UNKNOWN ISOMER)					C10. H14. O1
150	27577964	2-XYLYLETHANOL	981				C10. H14. O1
150	533186	O-CRESYL ACETATE	301	726	50		C9 . H10. O2
150	619647	P-ETHYLBENZOIC ACID			111	107	C9 . H10. O2
150	590023	BUTYL CHLOROACETATE					C6 . H11. O2 .CL1
151	2634335	1,2-BENZISOTHIAZOL-3(2H)-ONE		265			C7 . H5 . N1 . O1 . S1
151	934349	2(3H)-BENZOTHIAZOLONE	1054				C7 . H5 . N1 . O1 . S1
151	7214611	(1-NITROETHYL)BENZENE	936				C8 . H9 . N1 . O2
151	721461	~~(1-NITROETHYL)BENZENE~~ USE CAS NO. 7214611, ABOVE					C8 . H9 . N1 . O2
151	99514	1,2-DIMETHYL-4-NITROBENZENE	382				C8 . H9 . N1 . O2
151	27655261	3-HYDROXY-1,2-BENZISOTHIAZOLE			180		C7 . H5 . N1 . O1 . S1
152	1195795	FENCHONE	477	556			C10. H16. O1
152	76222	%CAMPHOR	363	356	149	114	C10. H16. O1
152	122598	PHENOXY ACETIC ACID	297	14	112		C8 . H8 . O3
152	100094	ANISIC ACID	246	572	54	110	C8 . H8 . O3
152	100438	1-UNDECYNE		823			C11. H20
152	2243983	5-UNDECYNE		824			C11. H20
152	89816	PIPERIDONE		860			C10. H16. O1
152	612204	2-(HYDROXYMETHYL)BENZOIC ACID	579	448			C8 . H8 . O3
152	83409	0-CRESOTIC ACID	1060				C8 . H8 . O3
152	579759	O-ANISIC ACID	433	482	173	109	C8 . H8 . O3
152	1197097	3',4'-DIHYDROXYACETOPHENONE	1057		89		C8 . H8 . O3
152	586389	3-METHOXYBENZOIC ACID	524	483			C8 . H8 . O3
152	547604	2,6,6-TRIMETHYL-BICYCLO[3.1.1]HEPTAN-3-ONE					C10. H16. O1
152	4695629	D-FENCHONE	784				C10. H16. O1
152	26532241	(3,3-DIMETHYLCYCLOHEXYLIDENE)ACETALDEHYDE					C10. H16. O1
152	4884246	[1,1'-BICYCLOPENTYL]-2-ONE			204		C10. H16. O1
152	551451	4-HYDROXY-3-METHYL-2-(2-PROPENYL)-2-CYCLOPENTEN-1-ONE	781				C9 . H12. O2
152	24955633	CIS-1,3-DICHLOROCYCLOHEXANE	549		11	168	C6 . H10.CL2
152	15932806	PULEGONE					C10. H16. O1
152	10292985	4,7,7-TRIMETHYLBICYCLO[2.2.1]HEPTAN-2-ONE	816				C10. H16. O1
152	121335	%VANILLIN					C8 . H8 . O3
152	567613	2-HYDROXY-6-METHYLBENZOIC ACID					C8 . H8 . O3
152	31600552	METHOXYMETHOXYMETHYLBENZENE					C9 . H12. O2
152	432257	2,6,6-TRIMETHYL-1-CYCLOHEXENE-1-CARBOXALDEHYDE	420				C10. H16. O1
152	90642	%MANDELIC ACID	745	52			C8 . H8 . O3

† SEE FOOTNOTE ON LAST PAGE

(Continued)

TABLE D1. (Continued)

WATER POLLUTANTS PAGE 23

IDENTIFIED COMPOUNDS BY MOLECULAR WEIGHT

NOTE--THIS LIST MAY CONTAIN COMPOUNDS THAT HAVE NOT BEEN FOUND IN ANY OF THE CONCENTRATES ANALYZED

MW	CAS NO.	COMMON NAME	DATA SET CORRELATION † DW	AWT	T4	T5	MOLECULAR FORMULA
152	621625	%2-CHLORO-1,1-DIETHOXYETHANE	111				C6 . H13. O2 .CL1
152	208968	ACENAPHTHYLENE		301			C12. H8
152	4501586	2,2,3-TRIMETHYL-3-CYCLOPENTENE-1-ACETALDEHYDE		480			C10. H16. O1
152	499741	6-METHYL-3-ISOPROPYL-2-CYCLOHEXEN-1-ONE		599			C10. H16. O1
152	2958761	2-METHYLDECALIN				24	C11. H20
152	2108921	1,1-DICHLOROCYCLOHEXANE			76	72	C6 . H10.CL2
152	822866	1,2-DICHLOROCYCLOHEXANE			239	21	C6 . H10.CL2
153	1984049	1-ISOCYANONAPHTHALENE	287		205		C11. H7 . N1
153	29559340	HEXAHYDRO-3-(2-PROPENYL)-2H-AZEPIN-2-ONE	743				C9 . H15. N1 . O1
154	92524	%BIPHENYL	170	346			C12. H10
154	470826	%CINEOLE	483	552			C10. H18. O1
154	124765	EXO-BORNEOL		354			C10. H18. O1
154	507700	%ENDO-BORNEOL	237	355			C10. H18. O1
154	586823	1-METHYL-4-(1-METHYLETHYL)-3-CYCLOHEXEN-1-OL		194			C10. H18. O1
154	513235	%THUJYL ALCOHOL		793			C10. H18. O1
154	10458147	MENTHONE	787	570			C10. H18. O1
154	1632731	FENCHYL ALCOHOL	234	357		138	C10. H18. O1
154	527	4-TERPINEOL ISOMER		198			C10. H18. O1
154	526	4-TERPINEOL ISOMER		136			C10. H18. O1
154	11039728	CIS-1,2-CIS-2,3-PLINOL		359			C10. H18. O1
154	99912	*P-CHLOROACETOPHENONE		1017			C8 . H7 . O1 .CL1
154	4840760	VINYL CYCLOHEXYLFORMATE		385			C9 . H14. O2
154	83329	%+ACENAPHTHALENE	995	744			C12. H10
154	821954	1-UNDELENE		252			C11. H22
154	98555	%ALPHA-TERPINEOL					C10. H18. O1
154	45955666	ETHENYL CYCLOPENTANEACETATE		282			C9 . H14. O2
154	16502888	4,4-DICHLOROBUTENOIC ACID	394	930			C4 . H4 . O2 .CL2
154	89861	BETA-RESORCYLIC ACID	928				C7 . H6 . O4
154	20547993	2,2,6-TRIMETHYL-1,4-CYCLOHEXANEDIONE	218	733	155		C9 . H14. O2
154	15404576	1,3,3,7-TETRAMETHYL-2-OXOBICYCLO[2.2.1]HEPTANE	312				C10. H18. O1
154	470677	1-METHYL-4-(1-METHYLETHYL)-7-OXABICYCLO[2.2.1]HEPTANE	473				C10. H18. O1
154	17983221	METHYL 2,2,3-TRIMETHYLCYCLOPENTYL KETONE	489				C10. H18. O1
154	2903233	2-METHYL-2-NONEN-4-ONE	723				C10. H18. O1
154	4099074	1,2-DIMETHYL-3-ISOPROPENYLCYCLOPENTANOL	785				C10. H18. O1
154	13509529	%1,3,6-TRIMETHYL-2,4(1H,3H)-PYRIMIDINEDIONE	1080				C7 . H10. N2 . O2
154	580992	3,5-DIMETHOXYPHENOL	272				C8 . H10. O3
154	54244892	4,5-DIETHYL-2,3-DIHYDRO-2,3-DIMETHYLFURAN	289				C10. H18. O1
154	532274	OMEGA-CHLOROACETOPHENONE					C8 . H7 . O1 .CL1
154	499767	2-METHLY-5-ISOPROPYLCYCLOHEXANONE	1032				C10. H18. O1
154	54244723	4-BUTYL-1,3-CYCLOPENTANEDIONE	749				C9 . H14. O2
154	1667645	2-CHLORO-1,3,5-TRIMETHYLBENZENE	655				C9 . H11.CL1
154	10482561	2-(4-METHYL-3-CYCLOHEXENYL)ISOPROPANOL		1104			C10. H18. O1
155	13861999	N-METHYLETHOSUXIMIDE		421			C8 . H13. N1 . O2
155	4419572	1-VALERYLPYRROLIDINE		870			C9 . H17. N1 . O1
156	569415	1,8-DIMETHYLNAPHTHALENE			196		C12. H12

† SEE FOOTNOTE ON LAST PAGE

(Continued)

TABLE D1. (Continued)

IDENTIFIED COMPOUNDS BY MOLECULAR WEIGHT

NOTE--THIS LIST MAY CONTAIN COMPOUNDS THAT HAVE NOT BEEN FOUND IN ANY OF THE CONCENTRATES ANALYZED

MW	CAS NO.	COMMON NAME	DATA SET CORRELATION †				MOLECULAR FORMULA
			DW	AWT	T4	T5	
156	581420	%2,6-DIMETHYLNAPHTHALENE	804	536			C12. H12
156	571584	%1,4-DIMETHYLNAPHTHALENE	1094	519			C12. H12
156	571619	1,5-DIMETHYLNAPHTHALENE					C12. H12
156	582161	2,7-DIMETHYLNAPHTHALENE		633			C12. H12
156	1127760	1-ETHYLNAPHTHALENE	406	955			C12. H12
156	1005	2-ACETYL-4-METHYL-4-PENTENOIC ACID		331			C8 . H12. O3
156	31642678	8-NONENOIC ACID		90			C4 . H16. O2
156	89781	%MENTHOL	235	790			C10. H20. O1
156	939275	%2-ETHYL NAPHTHALENE	452	518	195	96	C12. H12
156	581408	%2,3-DIMETHYLNAPHTHALENE		784			C12. H12
156	700	METHYL OCTENOATE		366			C9 . H16. O2
156	575439	1,6-DIMETHYLNAPHTHALENE	1071	537			C12. H12
156	573988	1,2-DIMETHYL NAPHTHALENE	2	975			C12. H12
156	300	DIMETHYL NAPHTHALENE	978	347			C12. H12
156	118912	O-CHLOROBENZOIC ACID	588	53			C7 . H5 . O2 .CL1
156	74113	%P-CHLOROBENZOIC ACID	514	43		177	C7 . H5 . O2 .CL1
156	708	CHLOROBENZOIC ACID ISOMER		375			C7 . H5 . O2 .CL1
156	741113	INVALID CAS NUMBER, SUBSTITUTE NUMBER 74113					C7 . H5 . O2 .CL1
156	575417	1,3-DIMETHYNAPHTHALENE	766	636	184		C12. H12
156	1370521	2-PHENYL-1,4-CYCLOHEXADIENE	418	1003			C12. H12
156	301	DIMETHYLNAPHTHALENE		397			C12. H12
156	575371	1,7-DIMETHYLNAPHTHALENE					C12. H12
156	535808	M-CHLOROBENZOIC ACID	637	123			C7 . H5 . O2 .CL1
156	820291	5-DECANONE		865			C10. H20. O1
156	624168	4-DECANONE		1029			C10. H20. O1
156	13491797	2-TERT-BUTYLCYCLOHEXANOL		279			C10. H20. O1
156	302	DIMETHYLNAPHTHALENE		635			C12. H12
156	13023002	2,2-DICHLOROBUTYRIC ACID	635	735			C4 . H6 . O2 .CL2
156	4794052	2,5-CYCLOHEXADIENYLBENZENE	457				C12. H12
156	106229	%BETA-CITRONELLOL	891				C10. H20. O1
156	1502052	CYCLODECANOL	908				C10. H20. O1
156	55013326	CIS-5-BUTYLDIHYDRO-4-METHYL-2(3H)-FURANONE	912				C9 . H16. O2
156	56052858	5-(PENTYLOXY)-2-PENTENE	492	602	190		C10. H20. O1
156	112312	%CAPRALDEHYDE	1081				C10. H20. O1
156	1120214	UNDECANE					C11. H24
156	123682	%2-PROPENYL HEXANOATE	537				C9 . H16. O2
156	1022	7-NONENOIC ACID	1041	679			C9 . H16. O2
156	3112854	METHYLSULFONYL BENZENE	370				C7 . H8 . O2 . S1
156	16519247	1-(2-PROPENYLOXY)HEPTANE	999	747			C10. H20. O1
156	13703521	(1,4-CYCLOHEXADIEN-1-YL)BENZENE		329			C12. H12
156	2518721	BARBITAL		931			C6 . H8 . N2 . O3
156	4124883	3-NONENOIC ACID					C9 . H16. O2
156	31502235	6-NONENOIC ACID		47			C9 . H16. O2
156	535159	ETHYL DICHLOROACETATE			217		C4 . H6 . O2 .CL2
156	22104809	2-DECEN-1-OL					C10. H20. O1

† SEE FOOTNOTE ON LAST PAGE

(Continued)

TABLE D1. (Continued)

IDENTIFIED COMPOUNDS BY MOLECULAR WEIGHT
NOTE--THIS LIST MAY CONTAIN COMPOUNDS THAT HAVE NOT BEEN FOUND IN ANY OF THE CONCENTRATES ANALYZED

MW	CAS NO.	COMMON NAME	DATA SET CORRELATION † DW	AWT	T4	T5	MOLECULAR FORMULA
157	761659	N,N-DI-N-BUTYL FORMAMIDE		195			C9 . H19. N1 . O1
157	121733	%M-CHLORONITROBENZENE	648	1002			C6 . H4 . N1 . O2 .CL1
157	877430	%2,6-DIMETHYLQUINOLINE		640			C11. H11. N1
157	1115964	N,N-DIMETHYLHEPTANAMIDE		137			C9 . H19. N1 . O1
157	7661474	7-ETHYLQUINOLINE		1023			C11. H11. N1
157	100005	P-CHLORONITROBENZENE	1095				C6 . H4 . N1 . O2 .CL1
157	88733	%O-CHLORONITROBENZENE	805	890			C6 . H2 . N1 . O2 .CL1
157	1721897	2-3-DIMETHYL QUINOLINE	701				C11. H11. N1
157	2623509	5,8-DIMETHYLQUINOLINE	1169				C11. H11. N1
157	1198374	%2,4-DIMETHYLQUINOLINE					C11. H11. N1
157	3434	3-HYDROXY-1,2-BENZISOTHIAZOLE		472			C7 . H5 . N1 . O1 . S1
157	16627353	N,N-DIETHYL-4-METHYL-2-PENTANAMINE				93	C10. H23. N1
158	4994165	4-PHENYLCYCLOHEXENE		512			C12. H14
158	112050	%PELARGONIC ACID	51	88	34		C9 . H18. O2
158	924163	%DI-N-BUTYLNITROSAMINE		977			C8 . H18. N2 . O1
158	2216695	METHOXYNAPHTHALENE		801			C11. H10. O1
158	504994	METHYLCAPRYLIC ACID		224			C9 . H18. O2
158	78693	TETRAHYDROLINALOOL		583			C10. H22. O1
158	3302123	2,2,4,4-TETRAMETHYL PENTANOIC ACID	23	248			C9 . H18. O2
158	60148949	2,6-DIMETHYLHEPTANOIC ACID	1127	642			C9 . H18. O2
158	41654095	2-ETHYL-3-METHYLMALEIC ACID	7	17	6	17	C7 . H10. O4
158	28098808	2-ETHYL-3-METHYLFUMARIC ACID	118	281			C7 . H10. O4
158	112061	HEPTYL ACETATE		875			C9 . H18. O2
158	4305264	6-(ACETYLOXY)-2-HEXANONE	256				C8 . H14. O3
158	1120065	2-DECANOL	877				C10. H22. O1
158	4749273	3,3,3-TRICHLORO-2-METHYLPROPENE					C4 . H5 .CL3
158	51149703	1-ETHOXY-2-HEPTANONE	885				C9 . H18. O2
158	112301	%N-DECYL ALCOHOL	441				C10. H22. O1
158	13279862	1,1,3-TRICHLORO-1-BUTENE					C4 . H5 .CL3
158	935455	2-ETHYL-2-ISOBUTYL-1,3-DIOXOLANE	511				C9 . H18. O2
158	56009360	2-METHOXY-4-METHYL-2-PENTENOIC ACID, METHYL ESTER	285				C8 . H14. O3
158	31702337	1,1,3-TRICHLORO-2-METHYL-1-PROPENE	1102				C4 . H5 .CL3
158	14112982	7-OXO-OCTANOIC ACID	1020	1071			C8 . H14. O3
158	3274291	2-ETHYLHEPTANOIC ACID	636	914			C9 . H18. O2
158	106309	%HEPTANOIC ACID,ETHYL ESTER	663				C9 . H18. O2
158	111115	METHYLCAPRYLATE	373				C9 . H18. O2
158	7469774	2-METHYL-1-NAPHTHALENOL	939				C11. H10. O1
158	2007	2-ETHYL-3-METHYL-2-BUTENEDIOIC ACID		681	56		C7 . H10. O4
158	3004931	2-METHYLCAPRYLIC ACID				174	C9 . H18. O2
158	16537125	3,3-DIMETHYL-2-(1-METHYLETHYL)BUTANOIC ACID					C9 . H18. O2
159	1640397	2,3,3-TRIMETHYL-3H-INDOLE		648			C11. H13. N1
159	3375846	3-(2-HYDROXYPROPYL)-5-METHYL-2-OXAZALIDINONE		691			C7 . H13. N1 . O3
160	1076615	6,7-DIMETHYL TETRALIN					C12. H16
160	1985597	1,1-DIMETHYL TETRALIN		183			C12. H16
160	54340884	1,5,7-TRIMETHYL INDAN		779			C12. H16

† SEE FOOTNOTE ON LAST

(Continued)

TABLE D1. (Continued)

IDENTIFIED COMPOUNDS BY MOLECULAR WEIGHT

NOTE--THIS LIST MAY CONTAIN COMPOUNDS THAT HAVE NOT BEEN FOUND IN ANY OF THE CONCENTRATES ANALYZED

MW	CAS NO.	COMMON NAME	DATA SET CORRELATION †				MOLECULAR FORMULA
			DW	AWT	T4	T5	
160	54340873	1,4,7-TRIMETHYL INDAN		965			C12. H16
160	6682060	4,5,7-TRIMETHYLINDAN		952			C12. H16
160	827521	PHENYLCYCLOHEXANE	1002	954			C12. H16
160	2044000	TETRAHYDROFURAN-2,5-DICARBOXYLIC ACID		207			C6 . H8 . O5
160	4839467	3,3 DIMETHYLGLUTARIC ACID		211			C7 . H12. O4
160	2613765	1,1,3-TRIMETHYL INDAN		969			C12. H16
160	25419334	1,8-DIMETHYL TETRALIN		974			C12. H16
160	13065071	2,7-DIMETHYL TETRALIN		534			C12. H16
160	61898586	3-METHYL ADIPIC ACID		837			C7 . H12. O4
160	681572	2,2-DIMETHYLGLUTARIC ACID	368	428			C7 . H12. O4
160	55724737	4-BUTOXYBUTYRIC ACID	331	451		179	C8 . H16. O3
160	56298750	1-ETHYL-1-METHYL INDAN					C12. H16
160	32367547	2-ETHYL TETRALIN	758			92	C12. H16
160	22531200	6-ETHYL TETRALIN	841				C12. H16
160	21564921	2,3-DIMETHYL TETRALIN	1062				C12. H16
160	2388149	4-ISOPROPYL-ALPHA-METHYL STYRENE					C12. H16
160	2568925	DI-SEC-BUTOXYMETHANE	903				C9 . H20. O2
160	918003	1,1,1-TRICHLORO-2-PROPANONE	110				C3 . H3 . O1 .CL3
160	620202	1-CHLORO-3-(CHLOROMETHYL)BENZENE	825				C7 . H6 .CL2
160	42775757	5-ETHYLTETRALIN					C12. H16
160	56282430	(1-CYCLOPROPYLISOPROPYL)BENZENE					C12. H16
160	16440374	5,6-DIMETHYL-1-INDANONE	197				C11. H12. O1
160	56667108	1-PHENYL-2-CYCLOPENTEN-1-OL					C11. H12. O1
160	54340895	1-(1,3-DIMETHYLBUTOXY)-2-PROPANOL	691				C9 . H20. O2
160	5004488	4-METHYL-1-PHTHALAZINONE	361				C9 . H8 . N2 . O1
150	1604111	METHYL SUCCINATE,DIMETHYL ESTER	661				C7 . H12. O4
160	14292274	3-HYDROXYOCTANOIC ACID	575			108	C8 . H16. O3
161	95761	%3,4-DICHLOROANILINE		410	249		C6 . H5 . N1 .CL2
161	608275	2,3-DICHLOROANILINE	344				C6 . H5 . N1 .CL2
161	554007	2,4-DICHLOROANILINE					C6 . H5 . N1 .CL2
161	23102025	4-METHYL-4-NITROPENTANOIC ACID		121	47		C6 . H15. N1 . O4
161	31030543	4-METHYL-4-NITROVALERIC ACID					C6 . H11. N1 . O4
161	4377359	2-(DICHLOROMETHYL)PYRIDINE					C6 . H5 . N1 .CL2
162	1985575	(1,1-DIMETHYLBUTYL) BENZENE	769	335			C12. H18
162	54410694	(3-METHYLPENTYL) BENZENE		960			C12. H18
162	19262205	(1,2,2-TRIMETHYLPROPYL) BENZENE		959			C12. H18
162	28080866	(2,2-DIMETHYLBUTYL) BENZENE		776			C12. H18
162	54410741	1-METHYL-2-(1-ETHYLPROPYL) BENZENE		960			C12. H18
162	19219853	(2-ETHYLBUTYL) BENZENE		961			C12. H18
162	99627	1,3-DISOPROPYL BENZENE		185			C12. H18
162	55669880	1,4-DIMETHYL-2-ISOBUTYL BENZENE	1012	953			C12. H18
162	6031023	2-PHENYLHEXANE		773			C12. H18
162	645136	4-ISOPROPYLACETOPHENONE	812	151			C11. H14. O1
162	54446785	1-(2-BUTOXYETHOXY) ETHANOL	384				C8 . H18. O3
162	1009616	DIACETYLBENZENE	120	795			C10. H10. O2

† SEE FOOTNOTE ON LAST PAGE

(Continued)

TABLE D1. (Continued)

IDENTIFIED COMPOUNDS BY MOLECULAR WEIGHT
NOTE--THIS LIST MAY CONTAIN COMPOUNDS THAT HAVE NOT BEEN FOUND IN ANY OF THE CONCENTRATES ANALYZED

MW	CAS NO.	COMMON NAME	DATA SET CORRELATION † DW	AWT	T4	T5	MOLECULAR FORMULA
162	54115	%NICOTINE	684	561			C10. H14. N2
162	645736	INVALID CAS NUMBER, SUBSTITUTE NUMBER 645136					C11. H14. O1
162	112367	BIS(2-ETHOXYETHYL)ETHER	854	206			C8 . H18. O3
162	250	C6-BENZENE		758			C12. H18
162	100185	P-DIISOPROPYL BENZENE	725	343			C12. H18
162	112345	2-(2-BUTOXYETHOXY)ETHANOL (A DIETHYLENE GLYCOL, MONO-BUTYL ETHER	79	4			C8 . H18. O3
162	120832	%*+$2,4-DICHLOROPHENOL	471	422	52		C6 . H4 . O1 .CL2
162	91587	%*+$2-CHLORONAPHTHALENE					C10. H7 .CL1
162	431	DIETHYLENE GLYCOL, BUTYL ETHER	116	39			C8 . H18. O3
162	1866393	P-TOLYL ACRYLIC ACID		862			C10. H10. O2
162	108850	%CYCLOHEXYL BROMIDE	277		245		C6 . H11.BR1
162	30393929	2,3-DIHYDRO-3,3-DIMETHYL-1H-INDEN-1-OL	1048				C11. H14. O1
162	877441	1,2,4-TRIETHYLBENZENE	442				C12. H18
162	102250	1,3,5-TRIETHYLBENZENE	424			91	C12. H18
162	55682730	2,2-DIMETHYL-3,5-DECADIYNE	455				C12. H18
162	4815570	P-DIPROPYLBENZENE	768				C12. H18
162	1483609	2,4-DIMETHYL-1-SEC-BUTYLBENZENE	762			28	C12. H18
162	22975582	P-(1-ETHYLPROPYL)TOLUENE	1138				C12. H18
162	2142656	O-ISOPROPYLACETOPHENONE	1149				C11. H14. O1
162	76039	%TCA (TRICHLOROACETIC ACID)	252				C2 . H1 . O2 .CL3
162	591355	%3,5-DICHLOROPHENOL	1074	916	51		C6 . H4 . O1 .CL2
162	75274	%BROMODICHLOROMETHANE	33		60	6	C1 . H1 .BR1 .CL2
162	42205083	1,2,3-TRIETHYLBENZENE					C12. H18
162	1077163	1-PHENYLHEXANE					C12. H18
162	20895447	4,6-DIMETHYLBENZOFURANONE					C10. H10. O2
162	1667012	2#,4#,6#-TRIMETHYLACETOPHENONE					C11. H14. O1
162	13524760	3,3-DIMETHYL-2(3H)-FURANONE	1034	1097			C10. H10. O2
162	583040	2-ALLYL BENZOATE					C10. H10. O2
162	5678	ALPHA-METHYLENE BENZENE PROPANOIC ACID		245			C10. H10. O2
162	2235838	5-PHENYL-2-PENTANONE		600			C11. H14. O1
162	2495394	2-BENZYLACRYLIC ACID		55			C10. H10. O2
162	583788	2,5-DICHLOROPHENOL			136		C6 . H4 . O1 .CL2
162	95772	3,4-DICHLOROPHENOL					C6 . H4 . O1 .CL2
163	524389	N-HYDROXYPHTHALAMIDE	160		165		C8 . H5 . N1 . O3
164	90277	2-PHENYLBUTYRIC ACID	523	100	156		C10. H12. O2
164	528985	2,4,5-TRIMETHYLBENZOIC ACID	431	125			C10. H12. O2
164	939480	ISOPROPYL BENZOATE	164	564			C10. H12. O2
164	536663	P-ISOPROPYL BENZOIC ACID	393	115	145		C10. H12. O2
164	112356	TRIETHYLENE GLYCOL METHYL ETHER	421	590			C7 . H16. O4
164	1821121	1-PHENYLBUTYRIC ACID	479	51			C10. H12. O2
164	480637	2,4,6-TRIMETHYLBENZOIC ACID	219	213			C10. H12. O2
164	1017	2-(2-(2-METHOXYETHOXY)ETHOXY)ETHANOL	1067				C7 . H16. O4
164	22084895	2-METHYLPHENYLPROPANOIC ACID	585				C10. H12. O2
164	98271	4-TERT-BUTYL-2-METHYLPHENOL	359	997			C11. H16. O1
164	3377875	3-HEXYL BROMIDE	1167				C6 . H13.BR1

† SEE FOOTNOTE ON LAST PAGE

(Continued)

TABLE D1. (Continued)

IDENTIFIED COMPOUNDS BY MOLECULAR WEIGHT
NOTE--THIS LIST MAY CONTAIN COMPOUNDS THAT HAVE NOT BEEN FOUND IN ANY OF THE CONCENTRATES ANALYZED

MW	CAS NO.	COMMON NAME	DATA SET CORRELATION † DW	AWT	T4	T5	MOLECULAR FORMULA
164	1076477	2,3,4-TRIMETHYLBENZOIC ACID	722				C10. H12. O2
164	2430042	O-ISOPROPYLBENZOIC ACID	1075		134		C10. H12. O2
164	2529364	2,3,6-TRIMETHYL BENZOIC ACID	727	239			C10. H12. O2
164	2437663	2,3,5-TRIMETHYLBENZOIC ACID					C10. H12. O2
164	101973	%BENZENEACETIC ACID,ETHYL ESTER	666				C10. H12. O2
164	56588400	CIS-2,3-DIHYDRO-2-METHYL-1H-INDENE-1,2-DIOL	1047				C10. H12. O2
164	127184	%ETHYLENE TETRACHLORIDE	415	1047			C2 .CL4
164	23617712	METHYL-2,4-DIMETHYL BENZOATE	343				C10. H12. O2
164	25081394	METHYL-3,5-DIMETHYL BENZOATE	136				C10. H12. O2
164	15012369	METHYL-2,3-DIMETHYL BENZOATE	990				C10. H12. O2
164	4346183	METHYL P-ETHYLBENZOATE	667		176	54	C10. H12. O2
164	103253	PHENYLPROPIONIC ACID,METHYL ESTER	378				C10. H12. O2
164	672764	2-HYDROXY-5-ISOPROPYL-2,4,6-CYCLOHEPTATRIEN-1-ONE					C10. H12. O2
164	103457	(2-PHENYLETHYL)ACETATE	980				C10. H12. O2
164	826551	BETA,BETA-DIMETHYLPHENYLACETIC ACID	846	244			C10. H12. O2
164	7495843	3-(P-TOLYL)PROPIONIC ACID				122	C10. H12. O2
164	7364207	METHYL P-ETHYLBENZOATE			169		C10. H12. O2
165	40991386	3-METHOXY-1,2-BENZISOTHIAZOLE	624	249			C8 . H7 . N1 . O1 . S1
165	5279141	(1-NITROPROPYL)BENZENE	207				C9 . H11. N1 . O2
165	17322348	2-NITROPROPYLBENZENE					C9 . H11. N1 . O2
165	10030781	1,7,DIHYDRO-2-(METHYLAMINO)-6H-PURIN-GONE	1052				C6 . H7 . N5 . O1
165	5325202	1,4-BENZOTHIAZIN-3-ONE		713	73		C8 . H7 . N1 . O1 . S1
165	55956291	4-ETHOXYETHYLANILINE			116		C10. H15. N1 . O1
166	86737	%+9H-FLUORENE	944	753			C13. H10
166	79345	%$1,1,2,2-TETRACHLOROETHANE	157	26			C2 . H2 .CL4
166	42058593	METHYL 3-HYDROXYPHENYLACETATE					C9 . H10. O3
166	100210	TEREPHTHALIC ACID	622	223			C8 . H8 . O4
166	88993	%PHTHALIC ACID	85	111	44	111	C8 . H6 . O4
166	93254	ANISOLE-2-ACETIC ACID		425			C9 . H10. O3
166	5368810	METHYL 3-METHOXYBENZOATE					C9 . H10. O3
166	55702540	3-CYCLOHEXYL-4-PENTEN-2-ONE	886	1025			C11. H18. O1
166	1013	2,6-DIMETHYLPHENOXY CARBONIC ACID		445			C9 . H10. O3
166	181157	SPIRODODECANE	1156				C12. H22
166	120149	VERATRALDEHYDE	765	698			C9 . H10. O3
166	4230324	BORNYL 2,5-DIKETONE	496				C10. H14. O2
166	55638501	2,2-DIMETHYL-3,5-DECADIENE	790				C12. H22
166	21293027	TRANS,CIS-4,5-DIETHYL-3,5-OCTADIENE	838				C12. H22
166	28017790	5,5-DIMETHYL-3-ISOPROPYL-2-CYCLOHEXENONE					C11. H18. O1
166	42180825	5-CHLORO-2-METHYLBENZOFURAN	1099				C7 . H7 . O1 .CL1
166	1008806	DECAHYDRO-2,3-DIMETHYLNAPHTHALENE	188				C12. H22
166	1618220	2,6-DIMETHYL DECALIN	425				C12. H22
166	1750512	1,6-DIMETHYL DECALIN	1007				C12. H22
166	1024	M-METHOXYPHENYL ACETATE		804			C9 . H10. O3
166	515300	.ALPHA.-HYDROXY-.ALPHA.-METHYL BENZENE ACETIC ACID	748	603			C9 . H10. O3
166	25551499	ETHYLDECALIN				26	C12. H22

† SEE FOOTNOTE ON LAST PAGE

(Continued)

TABLE D1. (Continued)

IDENTIFIED COMPOUNDS BY MOLECULAR WEIGHT

NOTE--THIS LIST MAY CONTAIN COMPOUNDS THAT HAVE NOT BEEN FOUND IN ANY OF THE CONCENTRATES ANALYZED

MW	CAS NO.	COMMON NAME	DATA SET CORRELATION †				MOLECULAR FORMULA
			DW	AWT	T4	T5	
166	1701775	METHOXY TOLUIC ACID				189	C9 . H10. O3
166	527184	1,4-DIHYDROXYTETRAMETHYLBENZENE			171		C10. H14. O2
166	203805	PHENALENE		1095			C13. H10
167	62237	%P-NITROBENZOIC ACID	929				C7 . H5 . N1 . O4
168	643583	2-METHYL BIPHENYL	171	755			C13. H12
168	101815	DIPHENYLMETHANE	403	782			C13. H12
168	58548382	METHYL ACENAPHTHENE (ISOMER UNKNOWN)		976			C13. H12
168	2469863	1-ALLYLNAPHTHALENE	850	1005	185		C13. H12
168	112414	ALPHA-DODECYLENE		253			C12. H24
168	16354953	1-PHENYL-1,2,3-PROPANETRIOL		267			C9 . H12. O3
168	10453891	CHRYSANTHEMIC ACID	548	280			C10. H16. O2
168	643936	3-METHYLBIPHENYL	209		199		C13. H12
168	3664640	4,8-DIMETHYL-7-NONEN-2-ONE	786				C11. H20. O1
168	54411039	3-METHYL-3-DECEN-2-ONE	901				C11. H20. O1
168	2648591	1,1-DICHLORO-2-HEXANONE	327				C6 . H10. O1 .CL2
168	2648604	4,4-DICHLORO-3-HEXANONE	328				C6 . H10. O1 .CL2
168	46005098	3-BUTYL-1,2,4-CYCLOPENTANETRIONE					C9 . H12. O3
168	40648268	1-TERT-BUTOXY-2-METHYLCYCLOHEXENE	1148				C11. H20. O1
168	132649	DIBENZOFURAN (DIPHENYLENE OXIDE)	634				C12. H8 . O1
168	121346	VANILLIC ACID					C8 . H8 . O4
168	53299539	(2-CHLORO-2-PROPENYL)OXYBENZENE	746				C9 . H9 . O1 .CL1
168	35692989	2-HYDROXY-3,5,5-TRIMETHYL-2-CYCLOHEXENE,1,4-DIONE	843				C9 . H12. O3
168	54410843	1-BROMO-2-CHLORO-2-BUTENE	941				C4 . H6 .BR1 .CL1
168	54411211	(1-CHLOROETHYL)DIMETHYLBENZENE	1162				C10. H13.CL1
168	4395793	2-CHLORO-P-CYMENE	947				C10. H13.CL1
168	644386	4-METHYL BIPHENYL			200		C13. H12
168	28645036	3-METHYLOCTAHYDROPENTALENE-1-CARBOXYLIC ACID		692			C10. H16. O2
168	33993349	4-HYDROXY-OCTAHYDRO-1-NAPHTHALENONE		693			C10. H16. O2
168	32511061	2,2-DIMETHYL-3-(2-METHYL-1-PROPENYL)CYCLOPROPANE CARBOXYLIC ACID		694			C10. H16. O2
169	122394	%*DIPHENYLAMINE	1083	7			C12. H11. N1
169	92671	%*4-PHENYLANILINE					C12. H11. N1
169	539037	N-(4-CHLOROPHENYL)ACETAMIDE				148	C8 . H8 . N1 . O1 .CL1
170	2027170	2-ISOPROPYLNAPHTHALENE		546			C13. H14
170	829265	2,3,6-TRIMETHYLNAPHTHALENE	1096	255	236		C13. H14
170	2245387	1,6,7-TRIMETHYLNAPHTHALENE	1097	520			C13. H14
170	3031081	1,3,6-TRIMETHYLNAPHTHALENE		256			C13. H14
170	317	TRIMETHYLNAPHTHALENE		785	131		C13. H14
170	318	C3 NAPHTHALENE		786			C13. H14
170	311	TRIMETHYLNAPHTHALENE		540	186	66	C13. H14
170	312	TRIMETHYLNAPHTHALENE		541			C13. H14
170	313	TRIMETHYLNAPHTHALENE		542			C13. H14
170	314	TRIMETHYLNAPHTHALENE		191			C13. H14
170	315	C3 NAPHTHALENE		767			C13. H14
170	316	TRIMETHYLNAPHTHALENE		768	201		C13. H14
170	325	N-PROPYLNAPHTHALENE		983			C13. H14

† SEE FOOTNOTE ON LAST PAGE

(Continued)

TABLE D1. (Continued)

IDENTIFIED COMPOUNDS BY MOLECULAR WEIGHT
NOTE--THIS LIST MAY CONTAIN COMPOUNDS THAT HAVE NOT BEEN FOUND IN ANY OF THE CONCENTRATES ANALYZED

MW	CAS NO.	COMMON NAME	DATA SET CORRELATION †				MOLECULAR FORMULA
			DW	AWT	T4	T5	
170	28652779	TRIMETHYLNAPHTHALENE (ISOMER UNKNOWN)					C13. H14
170	3876979	1,2,8-TRIMETHYLNAPHTHALENE (3,4,5-TRIME.NAP.)		634			C13. H14
170	319	TRIMETHYLNAPHTHALENE		984			C13. H14
170	17057919	1,3,8-TRIMETHYLNAPHTHALENE		411			C13. H14
170	90437	%2-HYDROXYBIPHENYL		399			C12. H10. O1
170	2131422	1,4,6-TRIMETHYL NAPHTHALENE	1098	413			C13. H14
170	2131411	1,4,5-TRIMETHYL NAPHTHALENE		1100			C13. H14
170	55402045	5,5-DIETHOXY-3-PENTYN-2-ONE	896				C9 . H14. O3
170	24588612	METHYL 3,6-DIHYDRO-4,5-DIMETHYL-2H-PYRAN-2-CARBOXYLATE	1146				C9 . H14. O3
170	101848	%PHENYL ETHER	1085	881	197	43	C12. H10. O1
170	16624069	2-CYCLOOCTYL-2-PROPANOL	488				C11. H22. O1
170	16782302	CYCLOOCTANEPROPANOL	499				C11. H22. O1
170	876277	4-CHLOROPHENYL ACETATE	638				C8 . H7 . O2 .CL1
170	14919541	CIS-3,4,4-TRIMETHYL-5-OXO-2-HEXENOIC ACID	532				C9 . H14. O3
170	108601	DICHLOROISOPROPYL ETHER	518				C6 . H12. O1 .CL2
170	1615061	1,3-DIHYDRO-2,2-DIOXIDE-2,1,3,BENZOTHIADIAZOLE	732				C6 . H6 . N2 . O2
170	927491	6-UNDECANONE	741				C11. H22. O1
170	5989333	5-ETHENYL TETRAHYDRO-.ALPHA.,.ALPHA.,5-TRIMETHYL-2FURANMETHANOL	1049	924			C10. H18. O2
170	106387	P-BROMOTOLUENE	945				C7 . H7 .BR1
170	3185997	P-METHYLSULFONYL TOLUENE	145				C8 . H10. O2 . S1
170	2806	3,7-DIMETHYL-6-OCTENOIC ACID		144			C10. H18. O2
170	14049117	TRIMETHYL-6-VINYLTETRAHYDROPYRAN-3-OL		926			C10. H18. O2
170	29253369	ISOPROPYLNAPHTHALENE			198		C13. H14
170	706149	5-HEXYLODIHYDROFURANONE			20	99	C10. H18. O2
170	5888	4-HYDROXY-3,3,5,5-TETRAMETHYLCYCLOHEXANONE					C10. H18. O2
170	54382586	3A,7A-DIMETHYL OCTAHYDRO-4-ISOBENZOFURANOL		1074			C10. H18. O2
171	70553	%P-TOLUENESULFONAMIDE		133	38		C7 . H9 . N1 . O2 . S1
171	10264172	N-HEXYLBUTANAMIDE		863			C10. H21. N1 . O1
171	827167	1,3,5-TRIMETHYLCYANURIC ACID	53		31	20	C6 . H9 . N3 . O3
171	89543	2-AMINO-5-CHLOROBENZOIC ACID		478			C7 . H6 . N1 . O2 .CL1
171	1364	TRIMETHYLQUINONE		1067			C12. H13. N1
171	2437721	2,3,4-TRIMETHYLQUINOLINE		1066			C12. H13. N1
172	334485	%CAPRIC ACID	82	72	110	156	C10. H20. O2
172	1731846	METHYL PELARGONATE	374				C10. H20. O2
172	31080372	2-METHYL-2-PROPYLHEXANOIC ACID	546	408			C10. H20. O2
172	4812297	3,6-DIMETHYLOCTANOIC ACID (AN ISODECANOIC ACID)	568	644		176	C10. H20. O2
172	2639636	HEXYL BUTYRATE		1033	10		C10. H20. O2
172	23708567	6-UNDECANOL	392		26		C11. H24. O1
172	112425	1-UNDECANOL	464				C11. H24. O1
172	80535	TERPIN	565	484			C10. H20. O2
172	93094	%2-NAPHTHOIC ACID	470	127			C11. H8 . O2
172	86555	1-NAPHTHOIC ACID	880	241			C11. H8 . O2
172	5336243	DMU (DIMETHYL UREA)	1137				C9 . H20. N2 . O1
172	31080394	2-PROPYLHEPTANOIC ACID	1073				C10. H20. O2
172	4506369	1,2-DIHYDRO-1,5,8-TRIMETHYLNAPHTHALENE					C13. H16

† SEE FOOTNOTE ON LAST PAGE

(Continued)

TABLE D1. (Continued)

IDENTIFIED COMPOUNDS BY MOLECULAR WEIGHT
NOTE--THIS LIST MAY CONTAIN COMPOUNDS THAT HAVE NOT BEEN FOUND IN ANY OF THE CONCENTRATES ANALYZED

MW	CAS NO.	COMMON NAME	DATA SET CORRELATION † DW	AMT	T4	T5	MOLECULAR FORMULA
172	33669760	1-METHYL-4-ISOPROPYL-1,2-CYCLOHEXANEDIOL	828				C10. H20. O2
172	1653301	2-HENDECANOL	463				C11. H24. O1
172	30316199	1,4-DIHYDRO-2,5,8-TRIMETHYLNAPHTHALENE					C13. H16
172	29304403	2-METHYL-3-OXOHEXANOIC ACID, ETHYL ESTER	813				C9 . H16. O3
172	54460990	4-ETHYL-2,6-DIMETHYL-4-HEPTANOL					C11. H24
172	93185	2-ETHOXYNAPHTHALENE	440				C12. H12. O1
172	6064524	4-OXO-NONANOIC ACID	688	461	83		C9 . H16. O3
172	2451016	~~NTERPIN~~ SEE CAS NO. 80535, PREVIOUS PAGE	~~565~~	~~488~~			~~C10. H20. O2~~
172	2177868	METHYL ISONONANOATE	672				C10. H20. O2
172	106321	XETHYL CAPRYLATE	673				C10. H20. O2
172	1731848	NONANOIC ACID,METHYL ESTER					C10. H20. O2
172	89634	P-CHLORO-2-NITROANILINE	954	609	139		C6 . H5 . N1 . N2 .CL1
172	119619	BENZOPHENONE					C13. H10. O1
172	2216811	HEPTYLPROPIONATE		1078			C10. H20. O2
172	2553960	4,6-DIMETHYL OCTANOIC ACID	300	920			C10. H20. O2
172	95567	O-BROMOPHENOL			70		C6 . H5 . O1 .BR1
172	28933597	ISOCAPRIC ACID					C10. H20. O2
172	26896208	ANTEISOCAPRIC ACID					C10. H20. O2
173	16067019	1-NITRO-2-OCTANONE	894				C8 . H15. N1 . O3
174	505486	SUBERIC ACID	87	91	72		C8 . H14. O4
174	55956257	DIPROPYLENE GLYCOL, 2-PROPENYL ETHER		116		144	C9 . H18. O3
174	22824324	1,4,6-TRIMETHYL TETRALIN		415			C13. H18
174	21693916	1,5,8-TRIMETHYL TETRALIN		398			C13. H18
174	29006062	METHYL 4-BUTOXYBUTYRATE		835			C9 . H18. O3
174	1018	BUTYL METHOXYBUTYRATE		140			C9 . H18. O3
174	1074119	(1,2-DICHLOROETHYL)BENZENE	647	829			C8 . H8 .CL2
174	2257354	2,3,3-TRICHLORO-2-PROPENOIC ACID	159	736	161		C3 . H1 . O2 .CL3
174	829992	1-HEPTENYLBENZENE	726				C13. H18
174	26447632	2-HEPTENYLBENZENE	168				C13. H18
174	4541133	4-(HEXYLOXY)-1-BUTANOL	31				C10. H22. O2
174	26447654	4-HEPTENYLBENZENE					C13. H18
174	123251	%DIETHYL SUCCINATE	367				C8 . H14. O4
174	13192046	2-KETOPENTANEDIOIC ACID, DIMETHYL ETHER	674				C7 . H10. O5
174	33796871	3-HYDROXYNONANOIC ACID	302	718	28	62	C9 . H18. O3
176	2132867	3-PHENYL-3-METHYLHEXANE		510			C13. H20
176	1943959	M-CYCLOHEXYLPHENOL		200			C12. H16. O1
176	486566	COTININE		571			C10. H12. N2 . O1
176	119426	O-CYCLOHEXYLPHENOL		638			C12. H16. O1
176	593715	CHLOROIODOMETHANE		853			C1 . H2 .CL1 . I1
176	29408420	1,6-DICHLORO-1,5-CYCLOOCTADIENE		1050			C8 . H10.CL2
176	13547063	1-CHLORO-4-(1-CHLOROETHENYL)CYCLOHEXENE					C8 . H10.CL2
176	5463503	4,7-DIMETHYL-1,3-ISOBENZOFURANDIONE	290				C10. H8 . O3
176	4468408	3-METHYL-3-PHENYLHEXANE					C13. H20
176	19961081	2,4,5-TRIETHYLTOLUENE					C13. H20
176	943271	P-TERT-BUTYLACETOPHENONE					C12. H16. O1

† SEE FOOTNOTE ON LAST PAGE

(Continued)

TABLE D1. (Continued)

IDENTIFIED COMPOUNDS BY MOLECULAR WEIGHT

NOTE--THIS LIST MAY CONTAIN COMPOUNDS THAT HAVE NOT BEEN FOUND IN ANY OF THE CONCENTRATES ANALYZED

MW	CAS NO.	COMMON NAME	DATA SET CORRELATION † DW	AWT	T4	T5	MOLECULAR FORMULA
176	19730042	2-(1-METHYL-2-PIPERIDINYL)-PYRIDINE	973				C11. H16. N2
176	86522	1-(CHLOROMETHYL)NAPHTHALENE	1164				C11. H9 .CL1
176	1076199	3,4-DIHYDROXY-6-METHOXY-1-NAPHTHALENONE		456			C11. H12. O2
176	14171892	6-PHENYL-2-HEXANONE		945			C12. H16. O1
176	6630019	1-T-BUTYL-3-ETHYL-5-METHYL BENZENE					C13. H20
178	120127	%+ANTHRACENE		380	242		C14. H10
178	2270204	5-PHENYL PENTANOIC ACID		182			C11. H14. O2
178	16433435	4-PHENYL PENTANOIC ACID	1115	31		125	C11. H14. O2
178	54518115	ISOPROPYL PHENYL PROPAN-1-OL		196			C12. H18. O1
178	85018	%+PHENANTHRENE	702	77			C14. H10
178	136607	BUTYLBENZOATE	522	489	193		C11. H14. O2
178	5669170	3-PHENYL PENTANOIC ACID	847	37		178	C11. H14. O2
178	7315686	3-METHYL-4-PHENYLBUTYRIC ACID	569	565			C11. H14. O2
178	112505	N-TRIETHYLENE GLYCOL, MONOETHYL ETHER	125	806			C8 . H18. O4
178	520	DIISOPROPYL PHENOL		539			C12. H18. O1
178	58443826	2-(2-ISOPROPYLPHENYL)-1-PROPANOL		360			C12. H18. O1
178	2078548	2,6-DIISOPROPYLPHENOL	913	409			C12. H18. O1
178	112492	TRIETHYLENE GLYCOL, DIMETHYL ETHER	775	395			C8 . H18. O4
178	2243358	2-ACETYLOXYACETOPHENONE	449				C10. H10. O3
178	20589859	1,2,3,3-TETRACHLORO-1-PROPENE	472				C3 . H2 .CL4
178	2934456	2,4-DIISOPROPYLPHENOL	1132	1088			C12. H18. O1
178	24142776	CUMENE ISOPROPYL ETHER	617				C12. H18. O1
178	54549723	P-(1-HYDROXY-1-METHYLETHYL)ACETOPHENONE	513	492			C11. H14. O2
178	17269942	1-TERT-BUTYL-4-ETHOXYBENZENE	503				C12. H18. O1
178	10226296	6-BROMO-2-HEXANONE	32	454			C6 . H11. O1 .BR1
178	1603798	ALPHA-OXOBENZENEACETIC ACID, ETHYL ESTER		731			C10. H10. O3
178	614277	.BETA.-OXO-BENZENEACETIC ACID, ETHYL ESTER	731				C10. H10. O3
178	13485660	4A,5,6,7,8,8A-HEXAHYDRO-4A,8A-DIMETHYL-2(1H)-NAPHTHALENONE(CIS)	198				C12. H18. O1
178	1974856	3-BROMOHEPTANE	866				C7 . H15.BR1
178	16824025	3-ETHOXY-1(3H)-ISOBENZOFURANONE		689			C10. H10. O3
178	667	2-(ETHYLPHENYL)PROPYL METHYL ETHER	414				C12. H18. O1
178	3333	4-PHENYL-4-OXO-BUTYRIC ACID		722			C10. H10. N3 . O3
178	4219550	O-PROPIONYL BENZOIC ACID		474			C10. H10. O3
178	28291692	N-ETHYL-2-BENZOTHIAZOLAMINE		902			C9 . H10. N2 . S1
178	1010486	BETA,BETA-DIMETHYLBENZENEPROPIONIC ACID		49			C11. H14. O2
178	824691	1,4-DICHLORO-2,5-DIHYDROXY BENZENE			137		C6 . H4 . O2 .CL2
178	5081	4-ETHYLTETRAMETHYLPHENOL			172		C12. H18. O1
178	15482549	2-ACETYL-P-TOLUIC ACID			23	124	C10. H10. O3
179	89521	N-ACETYLANTHRANILIC ACID					C9 . H9 . N1 . O3
179	34263644	3-ETHOXY-1,2-BENZISOTHIAZOLE					C9 . H9 . N1 . O1 . S1
179	15118602	P-AMINOBENZENE-T-BUTYRIC ACID		923			C10. H13. N1 . O2
180	2523377	9-METHYL-9H-FLUORENE					C14. H12
180	1430973	2-METHYL FLUORENE		787			C14. H12
180	120821	%*+$1,2,4-TRICHLOROBENZENE	354	840			C6 . H3 .CL3
180	776352	9,10-DIHYDROPHENANTHRENE		258			C14. H12

† SEE FOOTNOTE ON LAST PAGE

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TABLE D1. (Continued)

IDENTIFIED COMPOUNDS BY MOLECULAR WEIGHT

NOTE--THIS LIST MAY CONTAIN COMPOUNDS THAT HAVE NOT BEEN FOUND IN ANY OF THE CONCENTRATES ANALYZED

MW	CAS NO.	COMMON NAME	DATA SET CORRELATION † DW	AWT	T4	T5	MOLECULAR FORMULA
180	108703	%$1,3,5-TRICHLOROBENZENE					C6 . H3 .CL3
180	87616	$1,2,3-TRICHLOROBENZENE	645				C6 . H3 .CL3
180	15359996	BUTYLATED HYDROXY ANISOLE (BHA)		414			C11. H16. O2
180	54576419	BUTYL M-TOLYL SULFIDE		661			C11. H16. S1
180	4316238	4-METHYLPHTHALIC ACID	469	888	230		C9 . H8 . O4
180	18495302	1,1,2,3-TETRACHLOROPROPANE	818	944	246		C3 . H4 .CL4
180	103300	%STILBENE (TRANS)	411				C14. H12
180	1730376	1-METHYLFLUORENE	771	1052	207	117	C14. H12
180	588590	%STILBENE (CIS OR TRANS)	167				C14. H12
180	17092921	5,6,7,7A-TETRAHYDRO-4,4,7A-TRIMETHYL-2(4H)-BENZOFURANONE	248	688	101	116	C11. H16. O2
180	17138282	ETHYL 4-HYDROXYPHENYLACETATE	1133				C10. H12. O3
180	486259	%9H-FLUOREN-9-ONE	669		238	182	C13. H8 . O1
180	1131620	3',4'-DIMETHOXYACETOPHENONE	1082				C10. H12. O3
180	37102742	3-METHYLPHTHALIC ACID	481				C9 . H8 . O4
180	62338243	1-(4,5-DIETHYL-2-METHYL-1-CYCLOPENTEN-1-YL)ETHANONE	476				C12. H20. O1
180	15356748	5,6,7,7A-TETRAHYDRO-4,4,7A-TRIMETHYL-2(4H)-BENZOFURANONE	98	912			C11. H16. O2
180	530483	1,1-DIPHENYLETHENE					C14. H12
180	13116535	1,2,2,3-TETEACHLOROPROPANE	353				C3 , H4 .CL4
180	25013165	%P-METHOXY-T-BUTYL PHENOL		286			C11. H16. O2
181	615225	2-(METHYLTHIO)BENZOTHIAZOLE					C8 . H7 . N1 . S2
181	6967700	3-BUTYL-6-METHYL-2,4-PYRIDINEDIOL		287			C10. H15. N1 . O2
182	605390	2,2-DIMETHYL-1,1-BIPHENYL					C14. H14
182	78400	%TRIETHYL PHOSPHATE	97	567	94	139	C6 . H15. O4 . P1
182	600	DIMETHYL BIPHENYL		543			C14. H14
182	7383906	3,4'-DIMETHYL-1,1'-BIPHENYL	172	1006			C14. H14
182	2437561	1-TRIDECENE		404			C13. H26
182	14376820	1-BROMO-2-CHLOROCYCLOPENTANE		1022			C5 . H8 .BR1 .CL1
182	41654277	2-METHOXY-3,5,5-TRIMETHYL-2-CYCLOHEXENE-1,4-DIONE	436				C10. H14. O3
182	93072	VERATRIC ACID	205				C9 . H10. O4
182	91521	%2,4-DIMETHOXYBENZOIC ACID					C9 . H10. O4
182	612000	1,1-DIPHENYLETHANE	305				C14. H14
182	1812517	2-ETHYL-1,1-BIPHENYL	3	1051			C14. H14
182	92831	XANTHENE	904				C13. H10. O1
182	54346064	3A,4,5,7A-TETRAHYDRO-4-HYDROXY-3A,7A-DIMETHYL-1(3H)-ISO-BENZOFURANONE	915				C10. H14. O3
182	4645152	CYCLOHEXYL ETHER	835				C12. H22. O1
182	103297	SYM-DIPHENYLETHANE (BIBENZYL)	629				C14. H14
182	13019164	2-BUTYL-2-OCTENAL	1033				C12. H22. O1
182	7507893	1(2,6-DIHYDROXY-4-METHOXYPHENYL)ETHANONE	744				C9 . H10. O4
182	830137	CYCLODODECANOL	659				C12. H22. O1
182	121142	%1-METHYL-2,4-DINITROBENZENE	670		66	150	C7 . H6 . N2 . O4
182	51953167	1-ETHOXY DECALIN		460			C12. H22. O1
182	3021736	CIS-OCTAHYDRONAPHTHALENE CARBOXYLIC ACID		128			C11. H18. O2
182	4826624	2-DODECENAL			82		C12. H22. O1
182	613332	4,4-DIMETHYLBIPHENYL			203		C14. H14
182	612759	3,3-DIMETHYLBIPHENYL			202		C14. H14

† SEE FOOTNOTE ON LAST PAGE

(Continued)

TABLE D1. (Continued)

IDENTIFIED COMPOUNDS BY MOLECULAR WEIGHT
NOTE--THIS LIST MAY CONTAIN COMPOUNDS THAT HAVE NOT BEEN FOUND IN ANY OF THE CONCENTRATES ANALYZED

MW	CAS NO.	COMMON NAME	DATA SET CORRELATION †				MOLECULAR FORMULA
			DW	AMT	T4	T5	
182	686202	2,6-DINITROTOLUENE			65		C7 . H6 . N2 . O4
183	81072	%SACCHARIN	859	45			C7 . H5 . N1 . O3 . S1
183	56771507	PHENYL P-PYRIDYL KETONE					C12. H9 . N1 . O1
184	1134629	2-BUTYLNAPHTHALENE		342			C14. H16
184	1634099	1-BUTYLNAPHTHALENE		778			C14. H16
184	2876359	2-T-BUTYL NAPHTHALENE	1104	989			C14. H16
184	112389	10-UNDECENOIC ACID		504	22		C11. H20. O2
184	490653	1-METHYL-7-ISOPROPYL NAPHTHALENE	407	752			C14. H16
184	49622186	3,3,4-TRIMETHYLDECANE		805			C13. H28
184	17085915	1-TERT-BUTYLNAPHTHALENE		789			C14. H16
184	16727916	1-ISOBUTYLNAPHTHALENE		814			C14. H16
184	629505	TRIDECANE					C13. H28
184	54774899	2-METHYL-1-PROPYLNAPHTHALENE		990			C14. H16
184	54774946	BICYCLO[2.2.2]OCTANE-1,4-DIOL, MONOACETATE					C10. H16. O3
184	4354589	CYCLOHEXANEHEXANOL	319				C12. H24. O1
184	2499594	OCTYL ACRYLATE	542				C11. H20. O2
184	50639026	2-METHYL-5-UNDECANONE					C12. H24. O1
184	765059	DECYL VINYL ETHER	747				C12. H24. O1
184	34040647	4-CHLOROPHENYL ACETIC ACID, METHYL ESTER	952				C9 . H9 . O2 .CL1
184	1973224	1-BROMO-2-ETHYLBENZENE	643				C8 . H9 .BR1
184	1585075	1-BROMO-4-ETHYLBENZENE	350				C8 . H9 .BR1
184	104814	1-(BROMOMETHYL)-4-METHYLBENZENE	1159				C8 . H9 .BR1
184	27011467	1-CHLOROTRICYCLO[4.3.1.13.8]UNDECANE	653				C11. H17.CL1
184	35194399	ETHYLNONENOATE	375				C11. H22. O2
184	19780100	5-DODECANONE		899			C12. H24. O1
184	132650	DIBENZOTHIOPHENE		1045			C12. H8 . S1
184	104676	5-HEPTYL DIHYDRO-2-FURANONE			144		C11. H20. O2
184	530507	1,1-DIPHENYLHYDRAZINE					C12. H12. N2
185	640619	%N,4-DIMETHYLBENZENESULFONAMIDE	993	887			C8 . H11. N1 . O2 . S1
186	19377970	2,2,5,7-TETRAMETHYL-4,5-OCTADIENE-3-ONE		259			C12. H20. O1
186	112378	%N-UNDECYLIC ACID	1018	263	55		C11. H22. O2
186	33583027	2,5,8-TRIMETHYL-1-NAPHTHOL		654			C13. H14. O1
186	112583	DI-N-HEXYL ETHER		441			C12. H26. O1
186	112538	%LAURYL ALCOHOL	260	707	214		C12. H26. O1
186	1422260	9-KETOCAPRIC ACID	422	320	17		C10. H18. O3
186	112265	%ETHYLENE GLYCOL, BIS(2-CHLOROETHYL) ETHER	658				C6 . H12. O2 .CL2
186	6836380	6-DODECANOL	905				C12. H26. O1
186	10203288	2-DODECANOL	686				C12. H26. O1
186	110429	METHYL CAPRATE	376				C11. H22. O2
186	1534276	3-DODECANONE		1063			C12. H24. O1
186	19943716	4,6-DIMETHYLNONANOIC ACID		889			C11. H22. O2
186	3913028	2-BUTYLOCTANOL		605			C12. H26. O1
186	10203335	5-DODECANOL			135		C12. H26. O1
186	1119637	9-METHYLDECANOIC ACID					C11. H22. O2
186	5601685	ANTEISOUNDECANOIC ACID			120		C11. H22. O2

† SEE FOOTNOTE ON LAST PAGE

(Continued)

TABLE D1. (Continued)

IDENTIFIED COMPOUNDS BY MOLECULAR WEIGHT
NOTE--THIS LIST MAY CONTAIN COMPOUNDS THAT HAVE NOT BEEN FOUND IN ANY OF THE CONCENTRATES ANALYZED

MW	CAS NO.	COMMON NAME	DATA SET CORRELATION † DW	ANT	T4	T5	MOLECULAR FORMULA
188	33931689	4-ETHOXYBUTYL BUTANOATE		96			C10. H20. O3
188	20442062	2-BUTOXYETHYL BUTANOATE		98			C10. H20. O3
188	123999	%AZELAIC ACID	84	174	[illegible]	159	C9 . H16. O4
188	25961846	DIETHYLENEGLYCOL, CYCLOHEXYL ETHER		677			C10. H20. O3
188	23342258	2,2,5,7-TETRAMETHYL TETRALIN	213				C14. H20
188	2432793	THIOHEXANOIC ACID, S-BUTYL ESTER	490				C10. H20. O1 . S1
188	29518727	1-OCTENYLBENZENE					C14. H20
188	1603618	(2-CYCLOHEXYLETHYL)BENZENE					C14. H20
188	42044268	6-TERT-BUTYL TETRALIN					C14. H20
188	42044224	2-TERT-BUTYL TETRALIN					C14. H20
188	54789296	1-(DICHLOROMETHYL)-4-ETHYLBENZENE	807				C9 . H10.CL2
188	483556	PHTHIOCOL	750				C11. H8 . O3
188	5689123	1,1,3,3-TETRAMETHYL-2-INDANONE	146				C13. H16. O1
188	5393817	2-HYDROXY DECANOIC ACID		288			C10. H20. O3
188	14292263	3-HYDROXYCAPRIC ACID	848	126	91		C10. H20. O3
189	495692	N-BENZOYLGLYCINE (HIPPURIC ACID)		392			C9 . H9 . N1 . O3
190	33962139	1,4-DIETHYL-2,3,5,6-TETRAMETHYL BENZENE		777			C14. H22
190	3895178	2-ETHOXYETHYL-2-BUTOXYETHYL ETHER		557			C10. H22. O3
190	2189608	OCTYL BENZENE	1063	968			C14. H22
190	50840	2,4-DICHLOROBENZOIC ACID	793	142			C7 . H4 . O2 .CL2
190	51445	3,4-DICHLOROBENZOIC ACID	515	54	12		C7 . H4 . O2 .CL2
190	35075242	1-(3-BUTOXYPROPOXY)-2-PROPANOL (A DIPROPYLENE GLYCOL,*		656			C10. H22. O3
190	29911282	1-(2-BUTOXY-1-METHYLETHOXY)-2-PROPANOL (DIPROPYLENE **		435			C10. H22. O3
190	14128611	5-METHYL-5-PHENYL-2-HEXANONE	738	1028			C13. H18. O1
190	54789150	1-(1-ETHYLPROPYL)-2-PROPYLBENZENE	1005				C14. H22
190	33637286	TETRAETHYLBENZENE	405				C14. H22
190	1079965	N-DI-SEC-BUTYLBENZENE	860				C14. H22
190	52805842	1-[5-(2-FURANYLMETHYL)-2-FURANYL]ETHANONE					C11. H10. O3
190	18335154	3-PHENYLOCTANE					C14. H22
190	1014411	P-DI-SEC-BUTYLBENZENE	861				C14. H22
190	777220	2-PHENYLOCTANE					C14. H22
190	597637	TETRAETHYLGERMANE					C8 . H20
190	50793	2,6-DICHLOROBENZOIC ACID	525	473			C7 . H4 . O2 .CL2
190	17759885	2-BROMO-1,2-DICHLOROPROPANE	689	932			C3 . H5 .BR1 .CL2
190	33037079	1-BROMO-2,3-DICHLOROPROPANE	690				C5 . H5 .BR1 .CL2
190	36668458	3-BROMO-1,1-DICHLOROPROPANE	529				C3 . H5 .BR1 .CL2
190	5186685	4,6-DIISOPROPYL-M-XYLENE					C14. H22
191	3209221	1,2-DICHLORO-3-NITROBENZENE	946				C6 . H3 . N1 . O2 .CL2
191	611063	2,4-DICHLORO-1-NITROBENZENE	355		247		C6 . H3 . N1 . O2 .CL2
191	42498339	N-TERT-BUTYL-3-METHYLBENZAMIDE	288				C12. H17. N1 . O1
192	613127	%2-METHYL ANTHRACENE		788			C15. H12
192	779022	%9-METHYL ANTHRACENE		970	251		C15. H12
192	610480	1-METHYL ANTHRACENE		352			C15. H12
192	1638160	TRIPROPYLENE GLYCOL	692	114			C9 . H20. O4
192	59094712	4-METHYLPHENYLPENTANOIC ACID		612			C12. H16. O2
*BUTYL ETHER)		**GLYCOL,BUT.ET.)					

† SEE FOOTNOTE ON LAST PAGE

(Continued)

TABLE D1. (continued)

IDENTIFIED COMPOUNDS BY MOLECULAR WEIGHT
NOTE--THIS LIST MAY CONTAIN COMPOUNDS THAT HAVE NOT BEEN FOUND IN ANY OF THE CONCENTRATES ANALYZED

MW	CAS NO.	COMMON NAME	DATA SET CORRELATION †				MOLECULAR FORMULA
			DW	AWT	T4	T5	
192	832644	4-METHYLPHENANTHRENE	1056	892			C15. H12
192	1011	BETA,3,4-TRIMETHYLBENZENEPROPANOIC ACID		426			C12. H16. O2
192	5481213	4-TERT-BUTYL-O-PHENYLENE CYCLIC CARBONATE		423			C11. H12. O3
192	832713	%3-METHYLPHENANTHRENE	408	894			C15. H12
192	2049969	PENTYL BENZOATE	466	708			C12. H16. O2
192	1453061	(2,5-DIMETHYLBENZENE)BUTANOIC ACID		246	14		C13. H18. O2
192	127	4(2,5-XYLYL)BUTYRIC ACID		723			C12. H16. O2
192	24306238	GAMMA METHYLBENZENEBUTANOIC ACID, METHYL ESTER		994			C12. H16. O2
193	1205489	N-BENZOYLGLYCINE, METHYL ESTER	616				C10. H11. N1 . O3
193	2021207	3A,4,7,7A-TETRAHYDRO-2-PROPYL-1H-ISOINDOLE	919				C11. H15. N1 . O2
194	713462	2-(4-TERT-BUTYL PHENOXY)ETHANOL		193			C12. H18. O2
194	120616	$DIMETHYL TEREPHTHALATE		368			C10. H10. O4
194	58082	%CAFFEINE	474	313			C8 . H10. N4 . O2
194	131113	%$DIMETHYL PHTHALATE	345	197		169	C10. H10. O4
194	833818	ALPHA-METHYLSTILBENE	458				C15. H14
194	14064483	3-METHYLSTILBENE	1065				C15. H14
194	54824112	3A,4,7,7A-TETRAHYDRO-4,4,7-TRIMETHYL-1,3-ISOBENZOFURANDIONE					C11. H14. O3
194	94995	2,4-DICHLORO-1-(CHLOROMETHYL)BENZENE	942				C7 . H5 .CL3
194	102476	1,2-DICHLORO-4-(CHLOROMETHYL)BENZENE	943				C7 . H5 .CL3
194	3405600	1,2,3,4-TETRACHLOROBUTANE		893			C4 . H6 .CL4
194	4612639	DIMETHYLFLUORENE		891			C15. H14
194	626857	DIBUTYL SULFITE				154	C8 . H18. O3 . S1
195	634935	2,4,6-TRICHLOROANILINE	791	741			C6 . H4 . N1 .CL3
195	636306	2,4,5-TRICHLOROANILINE	351	882			C6 . H4 . N1 .CL3
196	947911	ACETYL BIPHENYL	983	95			C14. H12. O1
196	4821049	TERPENYL ACETATE		794			C12. H20. O2
196	88062	%*+$2,4,6-TRICHLOROPHENOL	36	163	49		C6 . H3 . O1 .CL3
196	2198756	*2,4-DICHLORONAPHTHALENE	649	1082			C10. H16.CL2
196	13540562	DIMETHYLDIPHENYLMETHANE		1010			C15. H16
196	425504541	ETHYLBENZYL BENZENE (ISOMER UNKNOWN)		1007			C15. H16
196	1120361	1-TETRADECENE		405			C14. H28
196	95954	%$2,4,5-TRICHLOROPHENOL		621			C6 . H3 . O1 .CL3
196	764938	INVALID CAS NUMBER, SUBSTITUTE NUMBER 76493					C12. H20. O2
196	76493	%BORNYL ACETATE		639			C12. H20. O2
196	36617024	(2-BROMOCYCLOPROPYL)BENZENE		858			C9 . H9 .BR1
196	4957146	DI-P-TOLYLMETHANE					C15. H16
196	4707500	6-PROPYL-BETA-RESORCYLIC ACID	123				C10. H12. O4
196	19420612	4-ISOPROPYL-O-PYROCATECHUIC ACID	124				C10. H12. O4
196	1016	C3-DIHYDROXYBENZOIC ACID	330				C10. H12. O4
196	1133835	LOLIOLIDE	932				C11. H16. O3
196	17619975	%STILBENE OXIDE	173			192	C14. H12. O1
196	5814857	1-METHYL-1,2-DIPHENYLETHANE	719				C15. H16
196	3976350	2,4,6-TRIMETHYLBIPHENYL					C15. H16
196	1015	ETHYL METHYL BIPHENYL					C15. H16
196	7180576	2-ISOVALERYL-4-METHYL-1,3-CYCLOPENTANEDIONE					C11. H16. O3

† SEE FOOTNOTE ON LAST PAGE

(continued)

TABLE D1. (Continued)

IDENTIFIED COMPOUNDS BY MOLECULAR WEIGHT
NOTE--THIS LIST MAY CONTAIN COMPOUNDS THAT HAVE NOT BEEN FOUND IN ANY OF THE CONCENTRATES ANALYZED

MW	CAS NO.	COMMON NAME	DATA SET CORRELATION †				MOLECULAR FORMULA
			DW	AWT	T4	T5	
196	496	P-PHENYLACETOPHENONE		78			C14. H12. O1
196	51422754	CIS-1-BROMO-2-CHLOROCYCLOHEXANE			77	75	C6 . H10.BR1 .CL1
197	15448994	N-METHYL SACCHARIN		807			C8 . H7 . N1 . O3 . S1
198	483783	1,6 DIMETHYL-4-ISOPROPYL-NAPHTHALENE	796	566			C15. H18
198	629594	%TETRADECANE		987			C14. H30
198	2382403	9-DODECENOIC ACID		647			C12. H22. O2
198	17663273	4,4,5,5-TETRAMETHYL-2,7-OCTANEDIONE	890				C12. H22. O2
198	13757989	6,7-DODECANEDIONE	237				C12. H22. O2
198	16409453	MENTHYL ACETATE	900				C12. H22. O2
198	54852754	[2-(PENTYLOXY)ETHYL]CYCLOHEXANE	924				C13. H26. O1
198	637978	2-IODOPENTANE					C5 . H11. I1
198	628171	1-IODOPENTANE					C5 . H11. I1
198	462180	7-TRIDECANONE	259				C13. H26. O1
198	93992	PHENYL BENZOATE					C13. H10. O2
198	7372885	4-METHYLDIBENZOTHIOPHENE		1046			C13. H10. S1
198	5079	4,5-DIMETHYLCYCLOOCTANE CARBOXYLIC ACID		122			C11. H20. O2
198	6885	2-CHLORO-P-TERT-BUTYLPHENOL					C11. H15. O1 .CL1
198	834140	ETHYLPHENOXYBENZENE		610			C14. H14. O1
198	7298104	ALPHA,4-DIHYDROXY-3-METHOXYPHENYLACETIC ACID					C9 . H10. O5
198	50113	1-METHYLBARBITAL					C9 . H14. N2 . O3
199	599699	N,N,4-TRIMETHYLBENZENESULFONAMIDE	261				C9 . H13. N1 . O2 .S1
199	1120167	DODECANAMIDE	989				C12. H25. N1 . O1
200	143077	%LAURIC ACID	86	84	35		C12. H24. O2
200	777957	CYCLIC TETRAMETHYLENE ADIPATE	399	217	104	100	C10. H16. O4
200	19094758	*METHYL CHLORO PHENOXYACETIC ACID (MCPA)					C9 . H9 . O3 .CL1
200	57289266	2-METHYL-1-DODECANOL	1139				C13. H28. O1
200	2575077	METHYL 9-OXODECANOATE	498				C11. H20. O3
200	50882638	1-BUTYL-2-NAPHTHALENOL					C14. H16. O1
200	50882616	2-BUTYL-1-NAPHTHALENOL					C14. H16. O1
200	110383	%ETHYL CAPRATE					C12. H24. O2
200	1731868	UNDECANOIC ACID,METHYL ESTER	665				C12. H24. O2
200	586765	P-BROMOBENZOIC ACID		719			C7 . H5 . O2 .BR1
200	676006	10-OXO-UNDECANOIC ACID		3		36	C11. H20. O3
200	6272384	2,4-DIHYDROXYDIPHENYL METHANE					C13. H12. O2
202	206440	%*+$FLUORANTHENE	933	322			C16. H10
202	129000	%+PYRENE	1198	164			C16. H10
202	3971333	2-ETHYLSUBERIC ACID		105			C10. H18. O4
202	111206	SEBACIC ACID	429	403			C10. H18. O4
202	483772	1,6-DIMETHYL-4-ISOPROPYL TETRALIN					C15. H22
202	16982006	P-(1,2,2-TRIMETHYLCYCLOPENTYL)TOLUENE					C15. H22
202	5921802	1,1-DIBUTOXY-BUTANE	808				C12. H26. O2
202	14629528	TRIETHYL(PENTYLOXY)SILANE					C11. H26. O1
202	17219215	2,2-DIMETHYLHEXANEDIOIC ACID, DIMETHYL ESTER	1036				C10. H18. O4
202	1732098	DIMETHYL SUBERATE	660				C10. H18. O4
204	1081772	1-PHENYL NONANE		535			C15. H24

† SEE FOOTNOTE ON LAST PAGE

(Continued)

TABLE D1. (Continued)

IDENTIFIED COMPOUNDS BY MOLECULAR WEIGHT
NOTE--THIS LIST MAY CONTAIN COMPOUNDS THAT HAVE NOT BEEN FOUND IN ANY OF THE CONCENTRATES ANALYZED

MW	CAS NO.	COMMON NAME	DATA SET CORRELATION †				MOLECULAR FORMULA
			DW	AWT	T4	T5	
204	6753986	ALPHA-CARYOPHYLLENE		376			C15. H24
204	13877935	BETA-CARYOPHYLLENE		221			C15. H24
204	469921	CLOVENE		228			C15. H24
204	17334553	BETA-GURJUNENE		225			C15. H24
204	61031729	ALPHA,ALPHA-DICHLOROPHENYLACETIC ACID		434			C8 . H6 . O2 .CL2
204	612942	2-PHENYLNAPHTHALENE	757				C16. H12
204	605027	1-PHENYLNAPHTHALENE	756				C16. H12
204	21460888	2,5-DICHLORO-4-METHYLBENZOIC ACID	879				C8 . H6 . O2 .CL2
204	18794948	7,11-DIMETHYL-3-METHYLENE-1,6,10-DODECATRIENE					C15. H24
205	133904	%AMIBEN	599				C7 . H5 . N1 . O2 .CL2
205	56961252	4-AMINO-3,5-DICHLOROBENZOIC ACID	597				C7 . H5 . N1 . O2 .CL2
206	3674757	9-ETHYL PHENANTHRENE		962			C16. H14
206	38275764	3-METHYL-4-(2.5-XYLYL) BUTANOIC ACID		748			C13. H18. O2
206	949133	2-OCTYLPHENOL		353			C14. H22. O1
206	20324338	TRIPROPYLENE GLYCOL, METHYL ETHER	581	66			C10. H22. O4
206	128392	2,6-DI-TERT-BUTYLPHENOL					C14. H22. O1
206	143226	TRIETHYLENE GLYCOL N-BUTYL ETHER		23			C10. H22. O4
206	140669	P-(1,1,3,3-TETRAMETHYLBUTYL)PHENOL		374		164	C14. H22. O1
206	406	TRIPROPYLENE GLYCOL, METHYL ETHER		67			C10. H22. O4
206	405	TRIPROPYLENE GLYCOL, METHYL ETHER		68			C10. H22. O4
206	404	TRIPROPYLENE GLYCOL, METHYL ETHER	243	64			C10. H22. O4
206	410	TRIPROPYLENE GLYCOL, METHYL ETHER					C10. H22. O4
206	411	TRIPROPYLENE GLYCOL, METHYL ETHER					C10. H22. O4
206	412	TRIPROPYLENE GLYCOL, METHYL ETHER					C10. H22. O4
206	413	TRIPROPYLENE GLYCOL, METHYL ETHER					C10. H22. O4
206	400	TRIPROPYLENE GLYCOL, METHYL ETHER	101	18	96	140	C10. H22. O4
206	401	TRIPROPYLENE GLYCOL, METHYL ETHER	203	21	97	141	C10. H22. O4
206	402	TRIPROPYLENE GLYCOL, METHYL ETHER	204	19	98	142	C10. H22. O4
206	403	TRIPROPYLENE GLYCOL, METHYL ETHER	102	20	99	143	C10. H22. O4
206	500	OCTYL PHENOL		601			C14. H22. O1
206	25498491	TRIPROPYLENE GLYCOL, METHYL ETHER (ISOMER UNKNOWN)		118			C10. H22. O4
206	10213771	TRIPROPYLENE GLYCOL, METHYL ETHER		285			C10. H22. O4
206	13133294	TRI-N-PROPYLENE GLYCOL, METHYL ETHER	1078	216			C10. H22. O4
206	54932784	P-(2,2,3,3-TETRAMETHYLBUTYL)PHENOL		234			C14. H22. O1
206	29681207	TRIETHYLENE GLYCOL, TERT-BUTYL ETHER		58			C10. H22. O4
206	7469401	1,2-DIHYDRO-4-PHENYLNAPHTHALENE	704				C16. H14
206	6789884	HEXYL BENZOATE	465				C13. H18. O2
206	124481	%DIBROMOCHLOROMETHANE	138		61	18	C1 . H1 .BR2 .CL1
206	96764	2,4-DI-TERT-BUTYLPHENOL	926				C14. H22. O1
206	55162839	5-(BENZOYLOXY)-PENTANAL					C12. H14. O3
206	55683108	TETRAMETHYLBENZENE PROPANOIC ACID	739				C13. H18. O2
206	30316144	2-METHYL-4-(2,5-XYLYL)BUTANOIC ACID	396				C13. H18. O2
207	7244679	N-BENZOYL-L-ALANINE, METHYL ESTER	867	941			C11. H13. N1 . O3
208	1798045	P-T-BUTYLPHENOXY ACETIC ACID		89			C12. H16. O3
208	34006774	$METHYL ETHYL PHTHALATE		97			C11. H12. O4

† SEE FOOTNOTE ON LAST PAGE

(Continued)

TABLE D1. (Continued)

IDENTIFIED COMPOUNDS BY MOLECULAR WEIGHT

NOTE--THIS LIST MAY CONTAIN COMPOUNDS THAT HAVE NOT BEEN FOUND IN ANY OF THE CONCENTRATES ANALYZED

MW	CAS NO.	COMMON NAME	DATA SET CORRELATION † DW	AWT	T4	T5	MOLECULAR FORMULA
208	10487920	ALPHA-METHYL-ALPHA-ACETYLOXYBENZENEACETIC ACID		653			C11. H12. O4
208	3018200	1-PHENYL TETRALIN	409				C16. H16
208	29422137	2-PHENYL TETRALIN	412				C16. H16
208	15404634	DECAHYDRO-1,4A-DIMETHYL-7-(1-METHYLETHYL)NAPHTHALENE					C15. H28
208	52588780	6,6-DIMETHYL-3,4-UNDECADIENE-2,10-DIONE	621				C13. H20. O2
208	41284882	6-PHENYL TETRALIN					C16. H16
208	54832836	OCTAHYDRO-2,2,4,4,7,7-HEXAMETHYL-1H-INDENE	541				C15. H28
208	84651	%9,10-ANTHRACENEDIONE	40				C14. H8 . O2
208	2316269	3-(3,4-DIMETHOXYPHENYL)-2-PROPENOIC ACID		242			C11. H12. O4
209	6267023	9,10-DIHYDRO-9,9-DIMETHYL ACRIDINE		93			C15. H15. N1
210	4920950	TETRAMETHYL BIPHENYL		949			C16. H18
210	87401	1,3,5-TRICHLORO-2-METHOXYBENZENE		833			C7 . H5 . O1 .CL3
210	13360617	1-PENTADECENE		406			C15. H30
210	26137531	1,2,3-TRIMETHYL-4-PROPENYLNAPHTHALENE (TRANS-ISOMER)	192	412			C16. H18
210	1142150	PARA-METHOXYSTILBENE		1015			C15. H14. O1
210	38171970	1-METHYL-4-(1-METHYL-2-BUTENYL)NAPHTHALENE	626				C16. H18
210	134816	BENZIL	1066				C14. H10. O2
210	18220901	ETHYL BENZOPHENONE					C15. H14. O1
210	626620	IODOCYCLOHEXANE	778				C6 . H11. I1
210	35194220	7,7-DIMETHYL-11-DODECEN-2-ONE	497				C14. H26. O1
210	2852688	BIS(3-METHYLPHENYL)METHANONE	1045				C15. H14. O1
210	61141660	3,4-DIETHYLBIPHENYL	60				C16. H18
210	26130847	CIS-1,2,3-TRIMETHYL-4-PROPENYLNAPHTHALENE	1100				C16. H18
210	54965536	2-CHLORO-1-(2,4-DIMETHYLPHENY)-2-METHYL-1-PROPANONE					C12. H15. O1 .CL1
210	2726218	1-1#-(1,2-DIMETHYL-1,2-ETHANEDIYL)BISBENZENE					C16. H18
210	55012696	2-CHLORO-1-(4-ETHYLPHENYL)-2-METHYL-1-PROPANONE	948				C12. H15. O1 .CL1
210	17180266	(DICHLOROMETHYL)NAPHTHALENE			244		C11. H8 .CL2
211	55030654	1,2,3,4-TETRAHYDRO-4,9-DIMETHYL ACRIDINE		774			C15. H17. N1
211	5650102	P-ISOPROPYLDIPHENYL AMINE		257			C15. H17. N1
212	629629	PENTADECANE					C15. H32
212	125406	BUTABARBITAL		424			C10. H16. N2 . O3
212	612351	2-(PHENYLMETHYL)BENZOIC ACID		427			C14. H12. O2
212	77281	1,3-DIMETHYL BUTABARBITAL		266			C10. H16. N2 . O3
212	1725048	OXACYCLOTETRADECAN-2-ONE	326				C13. H24. O2
212	6606344	4,4A,9,10-TETRAHYDRO-4A-METHYL-2(3H)-PHENANTHRENONE					C15. H16. O1
212	6262517	PENTACHLOROCYCLOPROPANE	519				C3 . H1 .CL5
212	2225403	3-METHYL-2,2-DIOXIDE-1H-2,1,3-BENZOTHIAPIAZIN-4(3H)-ONE	728				C8 . H8 . N2 . O3 . S1
212	10271575	1-CHLORO-2(PHENYLETHYNYL)BENZENE	656				C14. H9 .CL1
212	4478108	2-BROMO-4-METHYL-1-ISOPROPYLBENZENE	1163				C10. H13.BR1
213	3622842	N-BUTYLBENZENESULFONAMIDE	247	131			C10. H15. N1 . O2 . S1
214	93652	%2-(4-CHLORO-2-METHYLPHENOXY)PROPANOIC ACID				126	C10. H11. O3 .CL1
214	882097	CLOFIBRIC ACID	74	1	15	63	C10. H11. O3 .CL1
214	15104617	1,1,2,3,3-PENTACHLOROPROPANE	1069	1049			C3 . H3 .CL5
214	638539	TRIDECYLIC ACID	873	449	71		C13. H26. O2
214	131566	BENZORESORCINOL	81				C13. H10. O3

† SEE FOOTNOTE ON LAST PAGE

(Continued)

TABLE D1. (Continued)

IDENTIFIED COMPOUNDS BY MOLECULAR WEIGHT

NOTE--THIS LIST MAY CONTAIN COMPOUNDS THAT HAVE NOT BEEN FOUND IN ANY OF THE CONCENTRATES ANALYZED

MW	CAS NO.	COMMON NAME	DATA SET CORRELATION †				MOLECULAR FORMULA
			DW	AWT	T4	T5	
214	111820	METHYL LAURATE	342	906			C13. H26. O2
214	17413739	CLOFIBRIC ACID, M-CHLORO ISOMER	1019				C10. H11. O3 .CL1
214	95943	1,2,4,5-TETRACHLOROBENZENE	1161				C6 . H2 .CL4
214	26403145	ANTEISOTRIDECANOIC ACID			125		C13. H26. O2
214	25448242	ISO-TRIDECANOIC ACID			126		C13. H26. O2
214	7416571	10-METHYLDODECANOIC ACID					C13. H26. O2
214	5681961	11-METHYLDODECANOIC ACID					C13. H26. O2
214	5090	2-METHOXY-10-UNDECANOIC ACID					C12. H22. O3
214	214	2-METHOXY-10-UNDECENOIC ACID		911			C12. H22. O3
214	112721	MYRISTYL ALCOHOL		294			C14. H30. O1
215	1912249	%ATRAZINE	91				C8 . H14. N5 .CL1
216	2381217	1-METHYLPYRENE		349			C17. H12
216	1141384	2,6-NAPHTHALIC ACID		226			C12. H8 . O4
216	1852046	UNDECANEDIOIC ACID	526	450	175		C11. H20. O4
216	2084697	1,1,2,4,4,7-HEXAMETHYL TETRALIN					C16. H24
216	1732101	DIMETHYL AZELATE	358				C11. H20. O4
216	13523074	4-BROMO-2-METHOXY-5-METHYLPHENOL					C8 . H9 . O2 .BR1
218	613592	2-(PHENYLMETHYL) NAPHTHALENE		548			C17. H14
218	104723	1-PHENYL DECANE		190			C16. H26
218	142732	DIBUTYL DIETHYLENE GLYCOL; DIBUTYL #CARBITOL#					C12. H26. O3
218	6529539	1-(2-BROMOETHYL)-4-CHLOROBENZENE		855			C8 . H8 .BR1 .CL1
218	55591123	1,1-DIMETHYL INDAN-4-CARBOXYLIC ACID, ETHYL ESTER	448				C14. H18. O2
218	4955322	ALPHA-FARNESAL	914				C15. H22. O1
218	3373102	P-DI-TERT-PENTYLBENZENE					C16. H26
218	605016	PENTAETHYLBENZENE	333				C16. H26
218	218	TETRAETHYLENE GLYCOL MONOBUTYL ETHER		290			C12. H26. O3
219	90302	%*N-PHENYL-1-NAPHTHYLAMINE					C16. H13. N1
219	27356463	6-METHYL-2-PHENYLQUINOLINE		1030			C16. H13. N1
219	4789768	4-METHYL-2-PHENYLQUINOLINE		673			C16. H13. N1
219	6907591	1-(PHENYLMETHYL)ISOQUINOLINE		674			C16. H13. N1
220	3674735	2,3,5-TRIMETHYL PHENANTHRENE		351			C17. H16
220	719222	2,6-DI-T-BUTYL-P-BENZOQUINONE	792	169			C14. H20. O2
220	128370	BUTYLATED HYDROXY TOLUENE (BHT)	1084	34			C15. H24. O1
220	23189642	1,2,4-TRIMETHYL PHENANTHRENE		966			C17. H16
220	63018940	2,9,10-TRIMETHYL ANTHRACENE		967			C17. H16
220	20178341	TRIPROPYLENE GLYCOL, ETHYL ETHER ISOMER		199			C11. H24. O4
220	94757	%*2,4-DICHLOROPHENOXYACETIC ACID, (2,4-D)	427	270	85	128	C8 . H6 . O3 .CL2
220	25154523	NONYLPHENOL	1150	232		172	C15. H24. O1
220	11066492	ISONONYL PHENOL (ISOMER UNKNOWN)		588			C15. H24. O1
220	17404669	P-(1-METHYLOCTYL)PHENOL (A NONYL PHENOL)		589		165	C15. H24. O1
220	52427131	P-(1-ETHYL-1-METHYLHEXYL)PHENOL (A NONYL PHENOL)		386			C15. H24. O1
220	510	NONYL PHENOL ISOMER		826			C15. H24. O1
220	511	NONYL PHENOL ISOMER		991			C15. H24. O1
220	1918009	%DICAMBA	112	240	88		C8 . H6 . O3 .CL2
220	588227	%3,4-DICHLOROPHENOXYACETIC ACID	802				C8 . H6 . O3 .CL2

† SEE FOOTNOTE ON LAST PAGE

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TABLE D1. (Continued)

IDENTIFIED COMPOUNDS BY MOLECULAR WEIGHT

NOTE--THIS LIST MAY CONTAIN COMPOUNDS THAT HAVE NOT BEEN FOUND IN ANY OF THE CONCENTRATES ANALYZED

			DATA SET CORRELATION †				
MW	CAS NO.	COMMON NAME	DW	AMT	T4	T5	MOLECULAR FORMULA
220	711	DICHLOROPHENOXYACETIC ACID (ISOMER UNKNOWN)	253				C8 . H6 . O3 .CL2
220	54644405	2,2-DIMETHYLPROPANOIC ACID, 2,4,6-TRIMETHYLPHENYL ESTER	740				C14. H20. O2
220	4620477	3-HYDROXY-2,4-PENTANEDIONE,BENZOATE	1035				C12. H12. O4
221	1111	FLUOROIODOBENZENE (ISOMER UNKNOWN)		1098			C6 . H4 . F1 . I1
222	143248	TETRAETHYLENE GLYCOL DIMETHYLETHER	856	218			C10. H22. O5
222	84662	%+$DIETHYL PHTHALATE	37	69			C12. H14. O4
222	131704	%MONOBUTYL PHTHALATE	11	27	119	160	C12. H14. O4
222	54889984	P-TERT-BUTYLPHENOXYMETHYL ACETATE		134			C13. H18. O3
222	84548	%2-METHYLANTHRAQUINONE	759				C15. H10. O2
222	55332020	OCTAHYDRO-4A,5-DIMETHYL-3-(1-METHYLETHYL)-1(2H)-NAPHTHA*	240				C15. H26. O1
222	55332031	OCTAHYDRO-4A,5-DIMETHYL-3-ISOPROPYL-2(1H)-NAPHTHALENONE	782				C15. H26. O1
222	3790714	FARNESOL	1158				C15. H26. O1
222	54965434	3,5-T-BUTYL-4-HYDROXY-2,4-CYCLOHEXADIEN-1-ONE			208		C14. H22. O2
224	1335484	DIHYDRO FARNESOL		560			C15. H28. O1
224	629732	CETENE		407			C16. H32
224	1795160	DECYLCYCLOHEXANE					C16. H32
224	20195088	DIETHYL PENTYL PHOSPHATE	258				C9 . H21. O4 . P1
224	5085	FUMAROYL CHLORIDE			162		C4 . H2 . O2 .CL4
226	57432	%AMOBARBITAL	273	108			C11. H18. N2 . O3
226	76744	%PENTABARBITAL	274	212			C11. H18. N2 . O3
226	203123	BENZOFLUORANTHENE		781			C18. H10
226	56464965	6,6-DIMETHYL-2,5,10-UNDECANETRIONE	863				C13. H22. O3
226	7284162	TRIETHYLENE GLYCOL, PHENYL ETHER	1135				C12. H18. O4
226	2363715	HENEICOSANIC ACID	388	699			C21. H42. O2
228	218019	%*+CHRYSENE		775			C18. H12
228	28484222	2,4,6-TRIMETHYLUNDECANOIC ACID		503			C14. H28. O2
228	544638	%MYRISTIC ACID	18	73	37		C14. H28. O2
228	5574345	3,8-DIMETHYL-5-ISOPROPYL-1,2-NAPHTHOQUINONE		852			C15. H16. O2
228	106332	ETHYL LAURATE	211			157	C14. H28. O2
228	54812725	CYCLOHEXYLADIPATE					C12. H20. O4
228	7278651	3-7,11-TRIMETHYL-3-DODECANOL	707				C15. H32. O1
228	50397643	4-METHYLPHENYLSULFONYL ACETIC ACID, METHYLESTER	360				C10. H12. O4 . S1
228	55162419	CLOFIBRIC ACID,METHYL ESTER	675				C11. H13. O3 .CL1
228	1731880	METHYL ISOTRIDECANOATE	676				C14. H28. O2
228	543	ISOMYRISTIC ACID		319	53		C14. H28. O2
228	76937	ALPHA-HYDROXY-ALPHA-PHENYL PHENYL ACETIC ACID					C14. H12. O3
228	629765	1-PENTADECANOL					C15. H32. O1
228	634833	2,3,4,5-TETRACHLOROANILINE	937				C6 . H3 . N1 .CL4
230	26140603	TERPHENYL		350			C18. H14
230	58902	%$2,3,4,6-TETRACHLOROPHENOL		620			C6 . H2 . O1 .CL4
230	92068	M-TERPHENYL					C18. H14
230	20881043	1,2 3,5-BIS-O-(1-METHYLETHYLIDENE)-ALPHA-D-XYLOFURANOSE	238				C11. H18. O5
230	5414197	DI-(2-BROMOETHYL)ETHER	150				C4 . H8 . O1 .BR2
230	938227	2,3,4,6-TETRACHLOROPHENOL	639				C6 . H2 . O1 . CL4
230	693232	DODECANEDIOIC ACID		716			C12. H22. O4
		*LENONE					

† SEE FOOTNOTE ON LAST PAGE

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TABLE D1. (Continued)

IDENTIFIED COMPOUNDS BY MOLECULAR WEIGHT
NOTE--THIS LIST MAY CONTAIN COMPOUNDS THAT HAVE NOT BEEN FOUND IN ANY OF THE CONCENTRATES ANALYZED

MW	CAS NO.	COMMON NAME	DATA SET CORRELATION †				MOLECULAR FORMULA
			DW	ANT	T4	T5	
231	6806815	4,8,12-TRIMETHYL-3,7,11-TRIDECATRIENITRILE			81		C16. H25. N1
232	50066	XPHENOBARBITAL		101			C12. H12. N2 . O3
232	4536883	2-PHENYL UNDECANE		766			C17. H28
232	6742547	1-PHENYL UNDECANE		538			C17. H28
232	1003	DIETHYLENE GLYCOL, 2-METHOXYBUTYL BUTYL DIETHER		6			C13. H28. O4
232	2425549	1-CHLOROTETRADECANE					C14. H29.CL1
232	3144169	7,7-DIMETHYL-2-OXOBICYCLO[2.2.1]HEPTANE-1-METHANE SULFONIC ACID	41				C10. H16. O4 . S1
234	483658	XRETENE		547			C18. H18
234	4130421	2,6-BIS(1,1-DIMETHYLETHYL)-4-ETHYLPHENOL		159	212	170	C16. H26. O1
234	106376	*P-DIBROMOBENZENE					C6 . H4 .BR2
234	108361	M-DIBROMOBENZENE					C6 . H4 .BR2
234	583539	O-DIBROMOBENZENE					C6 . H4 .BR2
234	7343068	3,4,5,6-TETRAMETHYLPHENANTHRENE		856			C18. H18
234	7396385	2,4,5,7-TETRAMETHYLPHENANTHRENE		857			C18. H18
234	67721	PERCHLOROETHANE	642			73	C2 .CL6
234	54571488	2,4-DICHLOROPHENOXY ACETIC ACID, METHYL ESTER	671				C9 . H8 . O3 .CL2
234	25638146	BROMOCHLOROBENZOIC ACID		917			C7 . H4 . O2 .BR1 .CL1
234	5334792	1-BROMO-2,3-DIMETHYLNAPHTHALENE			206		C12. H11.BR1
236	3910358	1,1,3-TRIMETHYL-3-PHENYL INDAN		579	248		C18. H20
236	33508020	1,1,2-TRIMETHYL-3-PHENYL INDAN		815			C18. H20
236	33603393	1,2,3-TRIMETHYL-1-PHENYL INDAN (STERIOISOMER)		817			C18. H20
236	33611164	1,2,3-TRIMETHYL-1-PHENYL INDAN (STEREOISOMER)		818			C18. H20
236	34006763	$BUTYL METHYL PHTHALATE		57			C13. H16. O4
236	1004	$ISOBUTYL METHYL PHTHALATE		613			C13. H16. O4
236	1006	$SEC-BUTYL METHYL PHTHALATE		614			C13. H16. O4
236	1007	$TERT-BUTYL METHYL PHTHALATE		396			C13. H16. O4
236	21113553	1,1-DIPHENYLCYCLOHEXANE					C18. H20
236	25249392	BIS(CHLOROPHENYL)METHANE					C13. H10.CL2
236	128	2,5-DI(CHLOROMETHYL)-3-ETHYL BENZOIC ACID		724			C10. H14. O2 .CL2
236	1977958	1,5-BIS(T-BUTYL)-3,3-DIMETHYL BICYCLO[3.1.0]HEXAN-2-ONE		298		58	C16. H28. O1
236	23586643	1,1'-(3,3-DIMETHYL-1-BUTENYLIDENE)BISBENZENE			209		C18. H20
238	1023	1,1-BIS(O-ETHYLPHENYL)ETHANE	410				C18. H22
238	1027	1,1-BIS(M-ETHYLPHENYL)ETHANE	174				C18. H22
238	56667017	HEXAMETHYL BIPHENYL		950			C18. H22
238	6765395	1-HEPTADECENE	987	627			C17. H34
238	10224916	1,1-BIS(4-ETHYLPHENYL)ETHANE	165				C18. H22
238	57364791	4,4'-DIETHYLBIBENZYL	460				C18. H22
238	1021	ASYMMETRICAL BIS(ETHYLPHENYL)ETHANE					C18. H22
238	5396918	1,5-DIPHENYL-3-PENTANONE		883			C17. H18. O1
238	8895	DIBROMOCYCLOHEXENE	1123				C6 . H8 .BR2
239	739	BROMODICHLOROANILINE		1077			C6 . H4 . N1 .BR1 .CL2
240	4705344	4,4'-DIMETHOXYSTILBENE		797			C16. H16. O2
240	629787	HEPTADECANE					C17. H36
240	13183090	4-BROMO-3-PHENYLSYDNONE		857			C8 . H5 . N2 . O2 .BR1
240	106025	EXALTOLIDE					C15. H28. O2

† SEE FOOTNOTE ON LAST PAGE

(Continued)

TABLE D1. (Continued)

IDENTIFIED COMPOUNDS BY MOLECULAR WEIGHT

NOTE--THIS LIST MAY CONTAIN COMPOUNDS THAT HAVE NOT BEEN FOUND IN ANY OF THE CONCENTRATES ANALYZED

MW	CAS NO.	COMMON NAME	DATA SET CORRELATION † DW	AWT	T4	T5	MOLECULAR FORMULA
242	17465597	1,1,4,5,5,8-HEXAMETHYL-S-HYDRINDALENE		957			C18. H26
242	1002842	PENTADECANOIC ACID	19	74	174		C15. H30. O2
242	17465586	1,1,4,7,7,8-HEXAMETHYL-S-HYDRINDACENE		780			C18. H26
242	124107	METHYL MYRISTATE	127	493			C15. H30. O2
242	20273272	4-PHENYLBICYCLOHEXYL	1106	884	237		C18. H26
242	20273272	4-PHENYLBICYCLOHEXYL					C18. H26
242	21484127	CIS-4-PHENYLBICYCLOHEXYL					C18. H26
242	36653824	%CETYL ALCOHOL	708	326	59		C16. H34. O1
242	5502943	ANTEISOPENTADECANOIC ACID	339	284	90		C15. H30. O2
242	5129668	METHYL ANTEISOPENTADECANOATE	953				C16. H32. O2
242	637070	%CLOFIBRATE	668	831			C12. H15. O3 .CL1
242	544	ISOPENTADECANOIC ACID		161	84		C15. H30. O2
242	629823	DIOCTYLETHER			178		C16. H34. O1
242	2485714	8-METHYLMYRISTIC ACID					C15. H30. O2
243	3519877	METHYLBENZACRIDINE		1053			C18. H13. N1
244	42981760	2,6-DI-TERT-BUTYL TETRALIN		1020			C18. H28
244	2507553	2-HYDROXYTETRADECANOIC ACID	480				C14. H28. O3
244	1961724	3-HYDROXYTETRADECANOIC ACID	432	476			C14. H28. O3
244	28969108	METHYL VINYL MERCURY					C3 . H6 . HG1
246	1460022	1,3,5-TRI-TERT-BUTYL BENZENE		956			C18. H30
246	604886	HEXAETHYLBENZENE					C18. H30
246	14800169	1,2,4-TRIBUTYLBENZENE		135			C18. H30
246	1459116	1,2,4-TRITERTIARY BENZENE		1016			C18. H30
246	2719611	(1-METHYLUNDECYL)BENZENE			241		C18. H30
246	25265785	(1-PHENYLHEPTYL)BENZENE					C18. H30
248	4584638	2,5-DI-T-AMYL QUINONE		62			C16. H24. O2
248	1002	DIETHYLENE GLYCOL, 4-METHOXYBUTYL BUTYL DIETHER		5			C13. H28. O4
248	608935	PENTACHLOROBENZENE	1103				C6 . H1 .CL5
248	4361960	5-PHENYL-3(PHENYLMETHYLENE)-2(3H)-FURANONE					C17. H12. O2
248	1611923	3,5-DIBROMOTOLUENE	646				C7 . H6 .BR2
249	54571499	2,4-D, ETHYL ESTER	955				C10. H10. O3 .CL2
249	2176627	PENTACHLOROPYRIDINE		810			C5 . N1 .CL5
250	131168	$DI-N-PROPYL PHTHALATE	849	678			C14. H18. O4
250	75252	+%BROMOFORM	34		62	37	C1 . H1 .BR3
250	546	DIBROMOPHENOL		1102			C6 . H4 . O1 .BR2
278	611007	2,4-DIBROMOBENZOIC ACID		720			C7 . H4 . O2 .BR2
250	1376	TETRAPROPYLENE GLYCOL		901			C12. H26. O5
250	1377	TETRAPROPYLENE GLYCOL		709			C12. H26. O5
250	1378	TETRAPROPYLENE GLYCOL		710			C12. H26. O5
250	1379	TETRAPROPYLENE GLYCOL		711			C12. H26. O5
252	205992	%*+$3,4-BENZOFLUORANTHENE (B)					C20. H12
252	207089	%*+$11,12-BENZFLUORANTHENE (K)					C20. H12
252	50328	%*+$3,4-BENZPYRENE					C20. H12
252	112889	1-OCTADECENE		628			C18. H36
252	17844074	4-(1,5-DIMETHYL-3-OXOHEXYL)-1-CYCLOHEXENE-1-CARBOXYLIC ACID		56	164		C15. H24. O3

† SEE FOOTNOTE ON LAST PAGE

(Continued)

TABLE D1. (Continued)

IDENTIFIED COMPOUNDS BY MOLECULAR WEIGHT

NOTE--THIS LIST MAY CONTAIN COMPOUNDS THAT HAVE NOT BEEN FOUND IN ANY OF THE CONCENTRATES ANALYZED

MW	CAS NO.	COMMON NAME	DATA SET CORRELATION † DW	AWT	T4	T5	MOLECULAR FORMULA
254	93765	%*(2,4,5-TRICHLOROPHENOXY)ACETIC ACID	190	1034			C8 . H5 . O3 .CL3
254	593453	OCTADECANE		816			C18. H38
254	38963916	4-(1,5-DIMETHYL-3-OXOHEXYL)CYCLOHEXANECARBOXYLIC ACID	998	85	45	127	C15. H26. O3
254	2091294	PALMITOLEIC ACID	215	79	32		C16. H30. O2
254	373499	TRANS-9-HEXADECENOIC ACID	275	264			C16. H30. O2
254	575893	%2,4,6-TRICHLOROPHENOXYACETIC ACID					C8 . H5 . O3 .CL3
254	713	TRICHLOROPHENOXYACETIC ACID (ISOMER UNKNOWN)	528				C8 . H5 . O3 .CL3
254	254	1-[(2,6,6-TRIMETHYL-1-CYCLOHEXEN-1-YL)OXY]-1-BUTANOL ACETATE		289			C15. H26. O3
256	57103	%PALMITIC ACID	4	28			C16. H32. O2
256	7132641	METHYL PENTADECANOATE	631	742			C16. H32. O2
256	1454859	1-HEPTADECANOL	868	269			C17. H36. O1
256	124061	ETHYL MYRISTATE	187				C16. H32. O2
256	25323686	*TRICHLOROBIPHENYL		1035			C12. H7 .CL3
256	545	ISOPALMITIC ACID		321	87		C16. H32. O2
256	1119206	DIVINYL MERCURY			86	175	C4 . H6 . HG1
258	87683	%*+$HEXACHLORO-1,3-BUTADIENE	144				C4 .CL6
258	57345389	5-EPIDEOXYPODOCARPIC ACID	592	227			C17. H22. O2
258	30525894	POLYFORMALDEHYDE					C8 . H18. O9
258	105997	DIBUTYL ADIPATE					C14. H26. O4
258	56051606	DIBUTYL-3-METHYLGLUTARATE	753				C14. H26. O4
260	3650042	OCTAHYDRO-1,4A-DIMETHYL-1-PHENANTHRENE CARBOXILIC ACID,*	570	919	46		C17. H22. O2
260	23262795	1,2 5,6-BIS-O-ISOPROPYLIDENE-BETA-D-TALOFURANOSE	12	310			C12. H20. O6
260	20880937	1,2 4,5-DI-O-ISOPROPYLIDENE-ALPHA-D-FRUCTOPYRANOSE	13	293			C12. H20. O6
260	23262784	2,3 5,6-DI-O-ISOPROPYLIDENE-ALPHA-D-TALOFURANOSE	502				C12. H20. O6
262	27193868	DODECYL PHENOL					C18. H30
263	527208	*PENTACHLOROANILINE	352				C6 . H2 . N1 .CL5
264	20324349	TETRAPROPYLENE GLYCOL METHYL ETHER	857	803	102		C13. H28. O5
264	87865	%*+$PENTACHLOROPHENOL	423	162			C6 . H1 . O1 .CL5
266	126738	%TRIBUTYL PHOSPHATE	83	165	152	44	C12. H27. O4 . P1
266	5090415	9-OCTADECENAL	505				C18. H34. O1
266	107277	(CHLOROMETHYL)METHYL MERCURY					C2 . H5 .CL1 .HG1
268	629925	NONADECANE					C19. H40
268	7225663	7-HEXYLTRIDECANE					C19. H40
268	55000538	1,4-DIMETHYL-5-OCTYLNAPHTHALENE		1004			C20. H28
268	1120258	METHYL PALMITOLEATE		417			C17. H32. O2
268	5659416	2,3,4,5,5-PENTACHLORO-2,4-PENTADIENOIC ACID	594				C5 . H1 . O2 .CL5
268	3538944	2,4,5-TRICHLOROPHENOXY ACETIC ACID, METHYL ESTER	379				C9 . H7 . O3 .CL3
268	26265996	HEPTADECANOIC ACID			58		C17. H32. O2
270	77474	%*+$HEX (HEXACHLOROCYCLOPENTADIENE)					C5 .CL6
270	112390	METHYL PALMITATE	632	166	219		C17. H34. O2
270	506127	MARGARIC ACID	25	176			C17. H34. O2
270	41114005	ETHYL PENTADECANOATE	337				C17. H34. O2
270	1019	2-KETOPALMITIC ACID					C16. H30. O3
270	17670756	ETHYL 7-METHYLMYRISTATE	677				C17. H34. O2
270	55723938	7-METHYL-7-HEPTADECANOL	754				C18. H38. O1
		*METHYL ESTER					

† SEE FOOTNOTE ON LAST PAGE

(Continued)

TABLE D1. (Continued)

IDENTIFIED COMPOUNDS BY MOLECULAR WEIGHT
NOTE--THIS LIST MAY CONTAIN COMPOUNDS THAT HAVE NOT BEEN FOUND IN ANY OF THE CONCENTRATES ANALYZED

MW	CAS NO.	COMMON NAME	DATA SET CORRELATION †				MOLECULAR FORMULA
			DW	AWT	T4	T5	
270	5129602	METHYL ISOPALMITATE	633	1090			C17. H34. O2
270	457	ANTEISOHEPTADECANOIC ACID	997	175	57		C17. H34. O2
270	26762447	OCTADECANOL	996	500			C18. H38. O1
270	1713140	BUTYL CLOFIBRATE		311			C14. H19. O3 .CL1
272	506138	16-HYDROXY PALMITIC ACID		918			C16. H32. O3
276	191242	%*+$BENZ-(GHI)-PERYLENE					C22. H12
276	193395	%*+$INDENO(1,2,3-CD)PYRENE					C22. H12
276	30353594	HEXACHLOROPENTANE			78	145	C5 . H6 .CL6
278††	17851535	$N-BUTYL-ISOBUTYLPHTHALATE	76	94			C16. H22. O4
278	84742	%+$DI-N-BUTYLPHTHALATE	1	3			C16. H22. O4
278	84695	%$DI-ISOBUTYLPHTHALATE	20	81			C16. H22. O4
278	4986916	OCTADECATRIENOIC ACID		300	75		C18. H30. O2
306	129	2-METHYL-4-DIBROMOMETHYL BENZOIC ACID		475			C9 . H8 . O2 .BR2
280	2197526	8,11-OCTADECADIENOIC ACID		291	106		C18. H32. O2
281	301020	CIS-9-OCTADECENAMIDE	809				C18. H35. N1 . O1
282	112801	%OLEIC ACID	88	143	39		C18. H34. O2
282	118741	%*+$HEXACHLOROBENZENE		821			C6 .CL6
282	112958	EICOSANE					C20. H42
282	112798	ELAIDIC ACID	512	75			C18. H34. O2
282	693721	VACCENIC ACID	600	462			C18. H34. O2
282	593395	PETROSELINIC ACID	276				C18. H34. O2
284	57114	%STEARIC ACID	52	29			C18. H36. O2
284	115968	%TRIS-B-CHLOROETHYL PHOSPHATE	853	13			C6 . H12. O4 .CL3 . P1
284	2490495	METHYL ANTEISOHEPTADECANOATE		799			C18. H36. O2
284	1731926	METHYL HEPTADECANOATE (METHYL MARGARATE)	383	584			C18. H36. O2
284	628977	ETHYL PALMITATE	135	469	220	34	C18. H36. O2
284	52783434	NONADECANOL	242				C19. H40. O1
284	1731936	METHYL HEPTADECANOATE	934	1106			C18. H36. O2
284	24035505	OCTAHYDROPHENANTHRENE CARBOXALDEHYDE		885			C20. H28. O1
284	5630120	ISOSTEARIC ACID		696			C18. H36. O2
286	80079	SULFONYLBIS(4-CHLOROBENZENE)	152				C12. H8 . O2 .CL2 . S1
286	28984807	TRICHLOROHEPTAFLUOROBUTANE					C4 .CL3 . F7
288	58899	+%*$LINDANE	949	1037			C6 . H6 .CL6
288	319857	+%LINDANE (BETA ISOMER)	356				C6 . H6 .CL6
290	26914330	*$TETRACHLOROBIPHENYL	1165	1040			C12. H6 .CL4
290	41464408	*+$2,2≠,4,5≠-TETRACHLOROBIPHENYL					C12. H6 .CL4
292	1018	AMYL BUTYL PHTHALATE	510				C17. H24. O4
292	301008	METHYL-9,12,15-OCTADECATRIENOATE	992				C19. H32. O2
293	82688	%*PENTACHLORONITROBENZENE	357				C6 . N1 . O2 .CL5
294	13038476	METHYL-9,11-OCTADECADIENOATE	975	940			C19. H34. O2
296	13038454	METHYLOCTADEC-10-ENOATE	974	1009			C19. H36. O2
296	112629	METHYL OLEATE		80			C19. H36. O2
296	2462842	9-OCTADECENOATE (GEOMETRY UNKNOWN)					C19. H36. O2
296	1937628	METHYL ELIADATE		138			C19. H36. O2
296	52380333	METHYL-11-OCTADECENOATE	991				C19. H36. O2

† SEE FOOTNOTE ON LAST PAGE
†† 2,4-DIBROMOBENZOIC ACID (MW 278): LISTED IN MW 250 RANGE

(Continued)

TABLE D1. (Continued)

IDENTIFIED COMPOUNDS BY MOLECULAR WEIGHT
NOTE--THIS LIST MAY CONTAIN COMPOUNDS THAT HAVE NOT BEEN FOUND IN ANY OF THE CONCENTRATES ANALYZED

MW	CAS NO.	COMMON NAME	DATA SET CORRELATION †				MOLECULAR FORMULA
			DW	AWT	T4	T5	
298	112618	METHYL STEARATE	128	167	235		C19. H38. O2
298	14010232	ETHYL MARGARATE					C19. H38. O2
298	629969	ARACHIDYL ALCOHOL					C20. H42. O1
298	38411120	BUTYLBENZYLPHTHALATE	693	457			C18. H18. O4
298	625	DIDEHYDROGENATED ABIETIC ACID		490			C20. H26. O2
298	646300	NONADECANOIC ACID		463			C19. H38. O2
300	5155704	DEHYDROABIETIC ACID	59	76	8		C20. H28. O2
300	57983365	BIS(1-METHYLPROPYL) NONANEDIOATE					C17. H32. O4
302	2136790	2,3,5,6-TETRACHLOROTEREPHTHALIC ACID	140				C8 . H2 . O4 .CL4
302	624	ABIETIC ACID		740			C20. H30. O2
302	264	3-DICHLOPOMETHYL-4,6-DI-T-BUTYL-O-BENZOQUINONE		732			C15. H20. O2 .CL2
302	5835267	ISOPIMARIC ACID				193	C20. H30. O2
302	79549	LEVOPIMARIC ACID				171	C20. H30. O2
302	54307425	7-ETHENYLDODECAHYDRO-1,4A,7-TRIMETHYL-1-PHENANTHRENECAR=*					C20. H30. O2
302	6080	1,3-DIMETHYL-2-(2-ISOPROPYLPHENYL)ETHYLCYCLOHEXANE CAR- BOXILIC ACID	571			163	C20. H30. O2
304	4087696	HYDROGENATED ABIETIC ACID					C20. H32. O2
306††	131180	DIAMYLPHTHALATE	815				C18. H26. O4
310	849990	DICYCLOHEXYLADIPATE	788	373			C18. H30. O4
310	629970	DOCOSANE					C22. H46
312	506309	%ARACHIDONIC ACID		283			C20. H40. O2
312	1731940	METHYL NONADECANOATE		985			C20. H40. O2
312	85687	%+$BUTYL BENZYL PHTHALATE	292	158			C19. H20. O4
312	111615	ETHYL STEARATE	338			59	C20. H40. O2
312	3121	ISOEICOSANOIC ACID		697			C20. H40. O2
314	109433	DIBUTYL SEBACATE		192			C18. H34. O4
314	1235741	METHYLDEHYDROABIETATE		364			C21. H30. O2
314	110338	ADIPIC ACID, DIHEXYL ESTER	391	157	177	33	C18. H34. O4
314	110388	DIHEXYLADIPATE	341	59			C18. H34. O4
314	1759	HEXANEDIOIC ACID, DIHEXYL ESTER		1068			C18. H34. O4
315	38842147	2,3,4,5,6-PENTAFLUORO-N-(2-PHENYLETHYL)BENZAMIDE	459				C15. H10. N1 . O1 . F5
316	72559	%+$DDE		1043			C14. H8 .CL4
316	3424826	%O,P-DDE					C14. H8 .CL4
322	33374286	$BUTYL-BUTOXY ETHYL PHTHALATE		40			C18. H26. O5
322	1020	3-(2,3-DIBROMOPHENYL) PROPANOIC ACID					C9 . H8 . O2 .BR2
322	60333	9,12-OCTADECADIENOIC ACID		942			C21. H38. O2
324	25429292	*$PENTACHLOROBIPHENYL	1166				C12. H5 .CL5
324	638675	TRICOSANE					C23. H48
324	800	*+$PENTACHLOROBIPHENYL + OTHER PCBS	882	1041			C12. H5 .CL5
324	38380028	2,2≠,3,4,5≠-PENTACHLOROBIPHENYL					C12. H5 .CL5
326	115866	%*TRIPHENYL PHOSPHATE	810	1014			C18. H15. O4 . P1
326	18281044	ETHYL NONADECANOATE					C21. H42. O2
326	995	TRIS(CHLOROPROPYL)PHOSPHATE		145			C9 . H18. O4 .CL3 . P1
328	2001	2,4,6-TRIBROMOPHENOL,	38	721			C6 . H3 . O1 .BR3
330	84617	%$DICYCLOHEXYL PHTHALATE	703	82			C20. H26. O4
334	84753	%+$DIHEXYL PHTHALATE	265	1091			C20. H30. O4
		*BOXYLIC ACID					

† SEE FOOTNOTE ON LAST PAGE

†† 2-METHYL-4-DIBROMOMETHYLBENZOIC ACID, MW 306: LISTED IN MW 278 RANGE

(Continued)

TABLE D1. (Continued)

IDENTIFIED COMPOUNDS BY MOLECULAR WEIGHT
NOTE--THIS LIST MAY CONTAIN COMPOUNDS THAT HAVE NOT BEEN FOUND IN ANY OF THE CONCENTRATES ANALYZED

MW	CAS NO.	COMMON NAME	DATA SET CORRELATION † DW	AWT	T4	T5	MOLECULAR FORMULA
336	85701	%$BUTYL(BUTOXY CARBONYL) METHYL PHTHALATE		332			C18. H24. O6
338	646311	TETRACOSANE					C24. H50
340	6064900	METHYL HENEICOSANOATE		363			C22. H44. O2
340	55193798	METHYLTRIDECYLOCTANOATE		139			C22. H44. O2
340	119471	2,2#METHYLENEBIS(6-(1,1-DIMETHYLETHYL)-4-METHYLPHENOL)	1119				C23. H32. O2
340	25378261	BEHENIC ACID		464			C22. H44. O2
352	50293	%*+$DDT		1044			C14. H9 .CL5
352	629992	PENTACOSANE					C25. H52
354	2009	TRICOSANOIC ACID		582			C23. H46. O2
358	26601649	*$HEXACHLOROBIPHENYL		1042			C12. H4 .CL6
362	309002	%*+$ALDRIN					C12. H8 .CL6
366	630013	HEXACOSANE		819			C26. H54
366	366	DICYCLOHEXYL SEBACATE		485			C22. H38. O4
368	563042	*TRI-M-CRESYL PHOSPHATE		836			C21. H21. O4 . P1
368	1330785	*TRICRESYL PHOSPHATE (ISOMER UNKNOWN)		250			C21. H21. O4 . P1
368	557595	LIGNOCERIC ACID		292			C24. H48. O2
370	123795	DIOCTYL ADIPATE	129	24			C22. H42. O4
370	103231	%BIS(2-ETHYLHEXYL) ADIPATE	390	25			C22. H42. O4
370	76448	%*+$HEPTACHLOR	1107	1039			C10. H5 .CL7
370	541026	DECAMETHYLCYCLOPENTASILOXANE	654				C10. H30. O5
378	60571	%*+$DIELDRIN					C12. H8 . O1 .CL6
380	593497	HEPTACOSANE					C27. H56
382	506387	PENTACOSANOIC ACID		700			C25. H50. O2
390	117840	%+$DIOCTYLPHTHALATE	134	8			C24. H38. O4
390	117817	%+$BIS(2-ETHYLHEXYL) PHTHALATE	245	83			C24. H38. O4
390	27554263	DIISOOCTYLPHTHALATE	263	60			C24. H38. O4
396	55373892	METHYL PENTACOSANOATE	678				C26. H52. O2
396	506467	HEXACOSANOIC ACID		701			C26. H52. O2
406	5103742	1,2,4,5,6,7,8,8-OCTACHLORO-2,3,3A,4,7,7A-HEXAHYDRO-4,7-METHANOINDENE		702			C10. H6 .CL8
412	103242	DIOCTYL AZELATE	1134	299			C25. H48. O4
426	122623	DIOCTYL SEBACATE	435	2			C26. H50. O4
434	1806548	TRIOCTYL PHOSPHATE		362			C24. H51. O4 . P1
438	21641703	NONACHLOR		683			C10. H3 .CL9
444	540976	DODECAMETHYLCYCLOHEXASILOXANE	803				C12. H36. O6 .SI6
492	630079	PENTATRIACONTANE					C35. H72
540	2385855	%MIREX					C10.CL12
622	36355018	%*HEXABROMOBIPHENYL					C12. H4 .BR6

† THE NUMERICAL ENTRY IS THE SEQUENCE NUMBER OF THE RELEVANT TABLE AT WHICH THE COMPOUND CAN BE FOUND: DW AND AWT ARE THE DRINKING WATER AND ADVANCED WASTE TREATMENT WATER GROUPS OF CONCENTRATES IN TABLES 9 AND 10, RESPECTIVELY, OF VOLUME 1, AND TABLES 1(a AND b), RESPECTIVELY OF VOLUME 2. T4 AND T5 ARE THE CINCINNATI DW SAMPLES CORRESPONDING TO THE GAC CONTACTORS A AND D IN TABLES 5 AND 6, RESPECTIVELY, OF VOLUME 3.

APPENDIX E

HERL PROCEDURES FOR THE PREPARATION OF THE CINCINNATI, OHIO, OCTOBER 17, 1978 CONCENTRATES

HERL personnel prepared the three concentrates (T1C, T1X, and T1Y) of the Cincinnati, Ohio, October 17, 1978 sampling. These three concentrates were the only ones not produced by GSRI. Since the procedure used by HERL was somewhat different from that used by GSRI, the important differences are summarized here.

DW sampled from the laboratory tap was split into two streams of essentially equal flow of about 500 ml/min. One of the streams was used to fill 1510-liter capacity stainless steel reservoirs for later RO processing. The other stream was acidified to pH 2 with a metered flow of 6N HCL immediately before passage through a 25 cm by 3.2 cm column containing about 190 cc of XAD-2 resin. The flow rate and bed volume resulted in a mean column residency time of about 10 seconds. The XAD-2 resin had been prepared for use by consecutive Soxhlet extraction with methanol, acetonitrile, ethyl ether and methanol. The sampling at these specified rates required about 50 hours after which the XAD-2 resin was eluted with 450 ml of unpreserved distilled in glass grade diethyl ether. Volume reduction to about 10 ml by KD distillation produced concentrate T1Y.

Before beginning RO processing of the 1510-liter sample, the pH was adjusted to 4.3 by the addition of 0.52 ℓ of 6N HCl. In contrast to the GSRI RO processor (Figure 1), the HERL system was equipped with only the cellulose acetate RO unit. RO volume reduction proceeded until the brine was reduced to about 70 liters. Further volume reduction was accomplished by lyophilization to about 800 ml of liquid and about 500 ml of salts. The salts were removed by filtration and subjected to vacuum drying. The dry salts were extracted with pentane and methylene chloride aliquots that were reused in the extraction of the liquid. The 800 ml of liquid was extracted in the usual sequence (pentane, methylene chloride and, after acidification to pH 2, methylene chloride again), the extracts were combined and volume reduction to about 5 ml by KD distillation produced concentrate T1C. The extracted 800 ml of acidified brine was then passed through an XAD-2 resin column identical to the one described above for concentration by direct XAD-2 adsorption. The column was eluted with ethyl alcohol, as above, and final volume reduction to 10 ml produced concentrat T1X.

APPENDIX F

CONTENTS AND LISTS OF TABLES FOR VOLUMES 2 AND 3

The contents and lists of tables for the other volumes of this report are presented here to aid the reader's grasp of the scope of this report in the absense of these other two volumes.

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